

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
 Data File : BM047412.D
 Acq On : 30 Aug 2024 18:59
 Operator : RC/JU
 Sample : P3794-03
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 RT-857

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM047412.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.557	275	284	294	rVB	150394	224100	4.03%	0.382%
2	5.004	352	360	382	rBV	2534581	3897387	70.05%	6.650%
3	6.569	619	626	647	rBV	2301672	3880096	69.74%	6.621%
4	7.345	750	758	767	rBV	797916	1281165	23.03%	2.186%
5	8.492	946	953	975	rBV	1435693	2488737	44.73%	4.247%
6	10.098	1219	1226	1241	rBV	954755	1660930	29.85%	2.834%
7	10.869	1350	1357	1367	rBV	69565	166482	2.99%	0.284%
8	11.839	1517	1522	1527	rBV4	45629	89148	1.60%	0.152%
9	12.257	1589	1593	1598	rBV6	43930	96890	1.74%	0.165%
10	12.328	1600	1605	1611	rVV9	56646	132753	2.39%	0.227%
11	12.398	1612	1617	1622	rVB4	136015	226608	4.07%	0.387%
12	12.533	1636	1640	1642	rBV	90997	121059	2.18%	0.207%
13	12.569	1642	1646	1647	rVV2	102553	136114	2.45%	0.232%
14	12.610	1647	1653	1661	rVB	3233339	4903422	88.13%	8.367%
15	12.751	1672	1677	1682	rBV	208918	397099	7.14%	0.678%
16	13.316	1769	1773	1777	rBV4	157409	279640	5.03%	0.477%
17	13.404	1784	1788	1794	rVB	867486	1221874	21.96%	2.085%
18	13.504	1801	1805	1813	rBV6	293859	630918	11.34%	1.077%
19	13.727	1838	1843	1848	rBV4	453998	849822	15.27%	1.450%
20	13.822	1855	1859	1864	rVB	1106408	1561712	28.07%	2.665%
21	13.963	1879	1883	1886	rBV	447528	618299	11.11%	1.055%
22	14.004	1886	1890	1896	rVB	1605813	2443234	43.91%	4.169%
23	14.086	1901	1904	1912	rVV6	284407	493768	8.87%	0.843%
24	14.339	1944	1947	1951	rBV	347722	491070	8.83%	0.838%
25	14.557	1980	1984	1990	rBV3	897155	1349329	24.25%	2.302%
26	14.633	1994	1997	1998	rBV2	328041	361198	6.49%	0.616%
27	14.727	2010	2013	2020	rBV4	401735	774697	13.92%	1.322%
28	14.798	2021	2025	2031	rVV	1693589	2334548	41.96%	3.984%
29	15.521	2143	2148	2153	rBV2	2658133	4299859	77.29%	7.337%
30	15.763	2186	2189	2191	rBV2	877224	1203742	21.64%	2.054%
31	15.792	2191	2194	2198	rVB	2346963	3051122	54.84%	5.206%
32	16.621	2331	2335	2341	rVB	3459106	5194115	93.36%	8.863%
33	16.780	2359	2362	2365	rBV	1233771	1570136	28.22%	2.679%
34	19.445	2811	2815	2826	rVB	4282108	5563606	100.00%	9.494%
35	21.021	3079	3083	3087	rVB	1581842	2029133	36.47%	3.462%
36	23.721	3535	3542	3553	rVB	1114397	2579410	46.36%	4.401%

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047412.D
Acq On : 30 Aug 2024 18:59
Operator : RC/JU
Sample : P3794-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RT-857

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

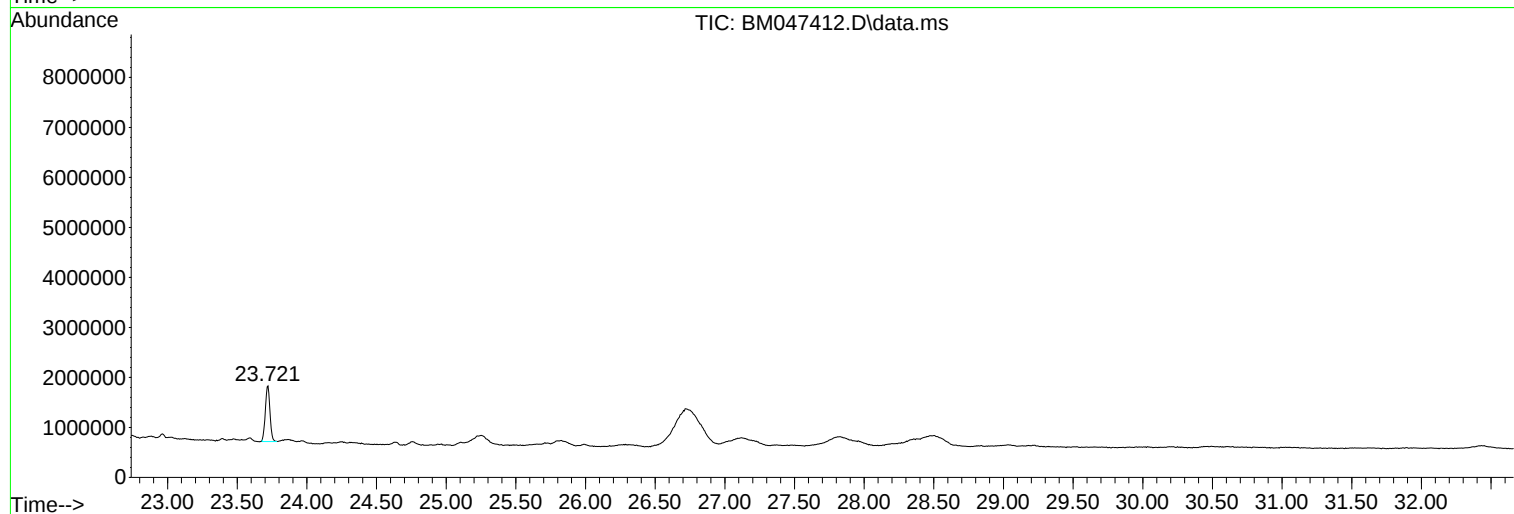
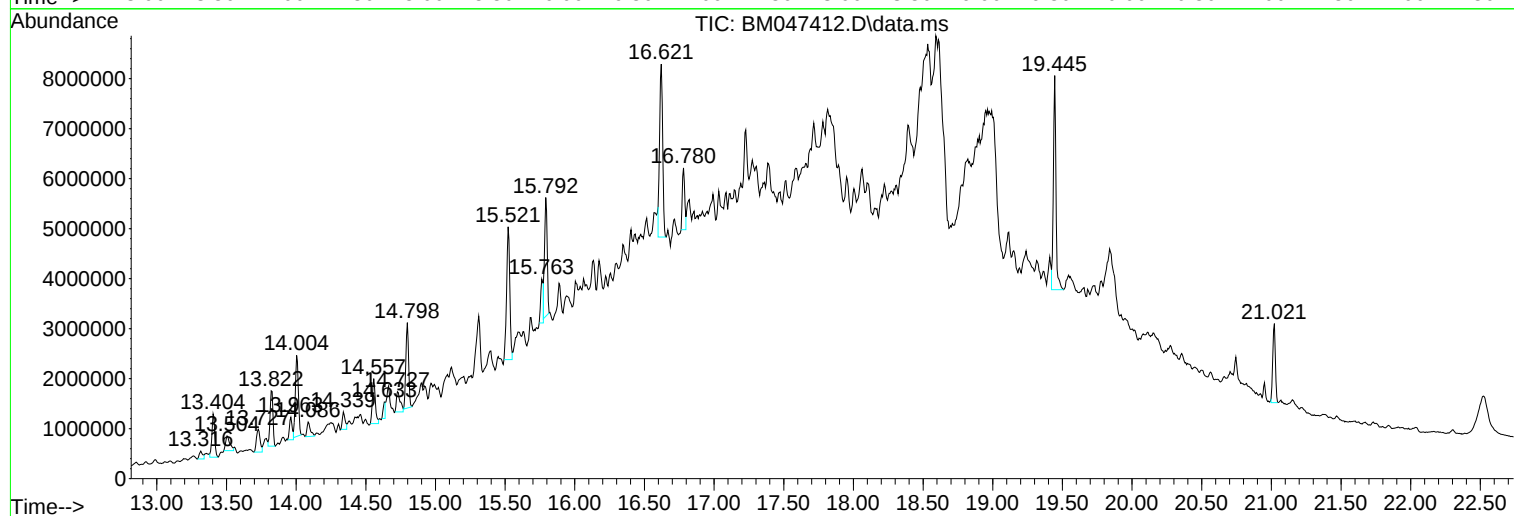
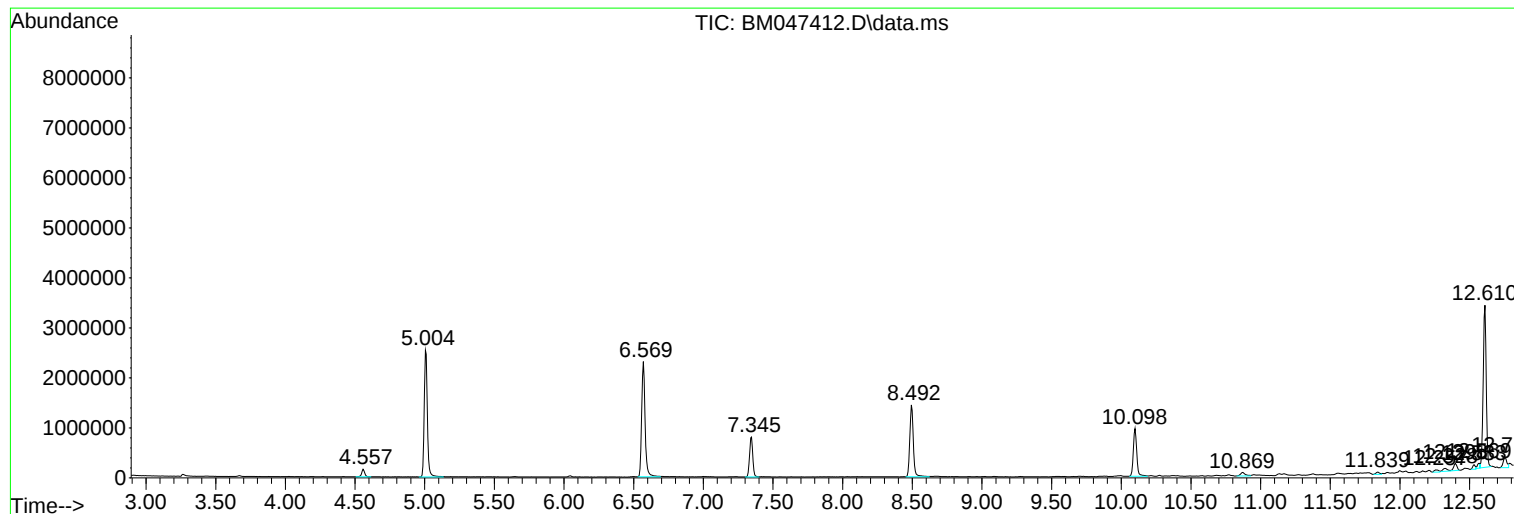
Sum of corrected areas: 58603222

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047412.D
Acq On : 30 Aug 2024 18:59
Operator : RC/JU
Sample : P3794-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RT-857

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047412.D
Acq On : 30 Aug 2024 18:59
Operator : RC/JU
Sample : P3794-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RT-857

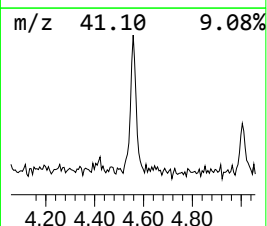
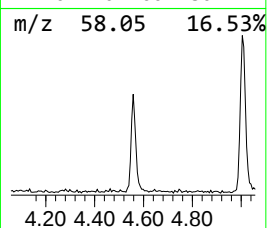
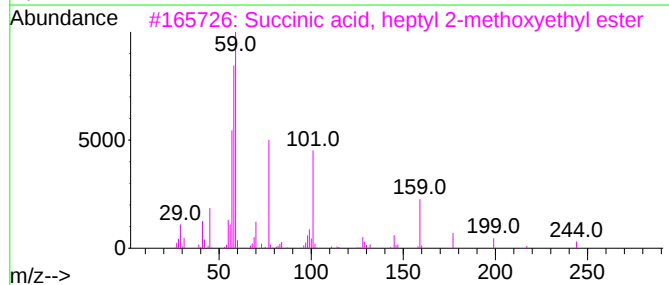
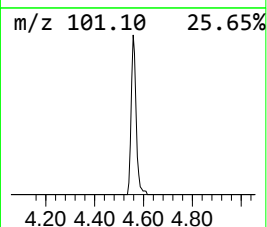
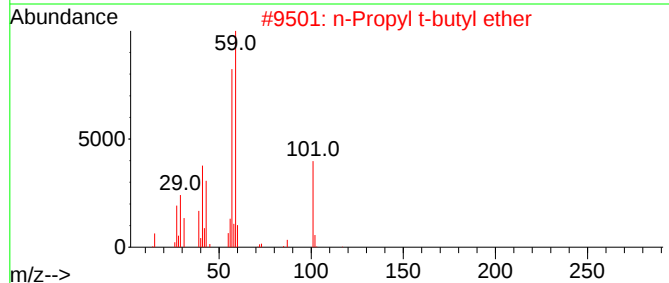
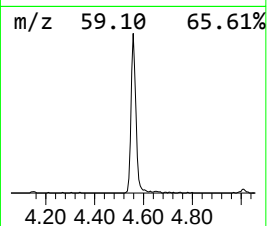
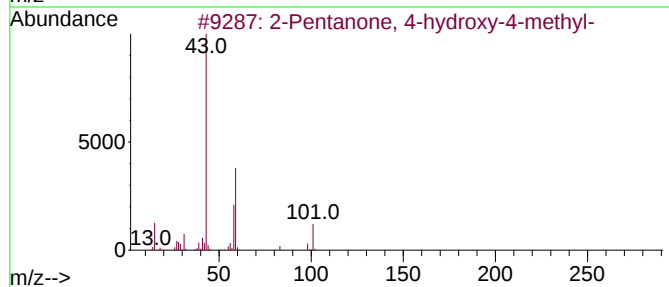
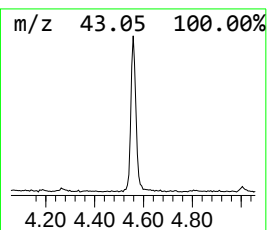
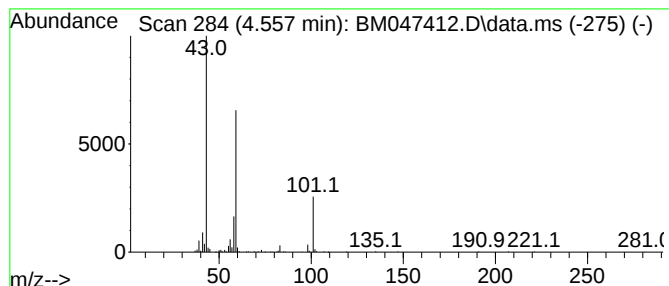
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.557	3.50 ng	224100	1,4-Dichlorobenzene-d4	7.345

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33
3			Succinic acid, heptyl 2-methoxye...	274	C14H26O5	1000325-80-7	33
4			Tetraglyme	222	C10H22O5	000143-24-8	32
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047412.D
Acq On : 30 Aug 2024 18:59
Operator : RC/JU
Sample : P3794-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RT-857

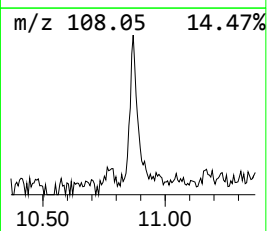
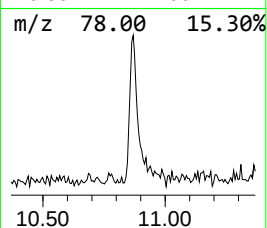
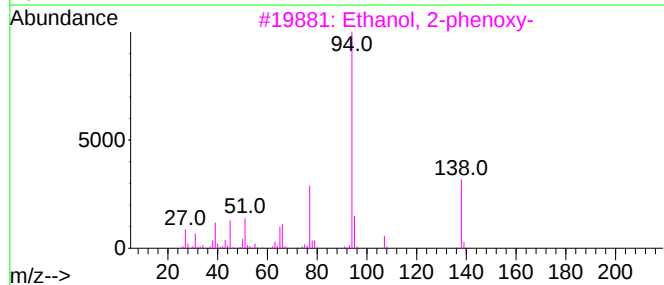
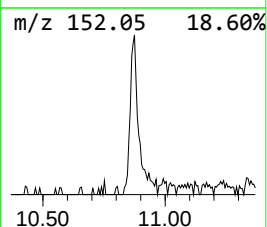
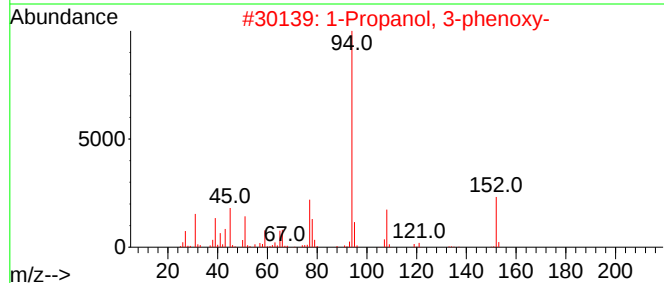
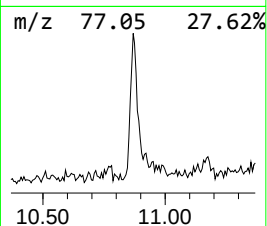
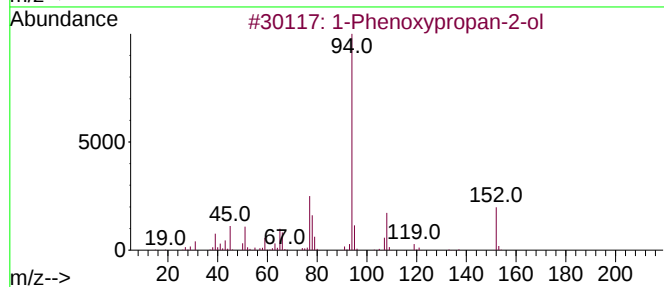
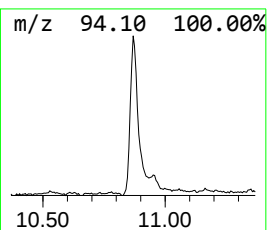
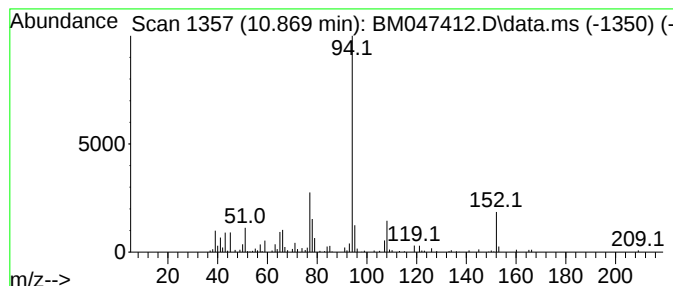
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1-Phenoxypropan-2-ol Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.869	2.00 ng	166482	Naphthalene-d8	10.098

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2		1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	87
3		Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4		1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
5		1-Phenoxy-2-chloropropane	170	C9H11ClO	053491-30-8	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047412.D
Acq On : 30 Aug 2024 18:59
Operator : RC/JU
Sample : P3794-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RT-857

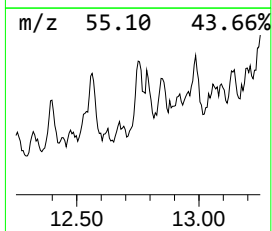
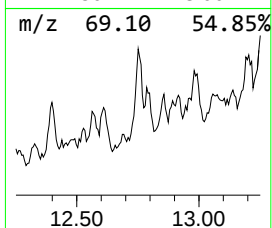
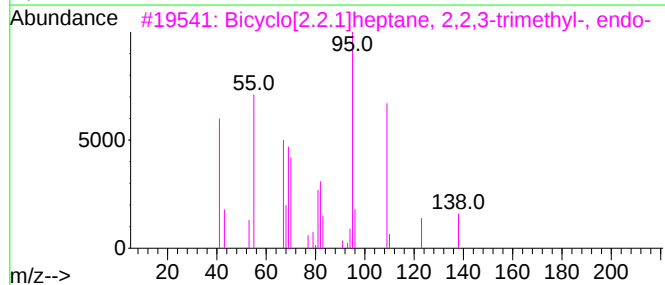
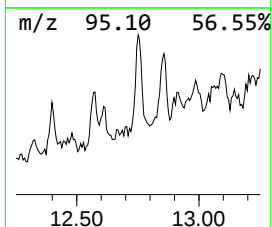
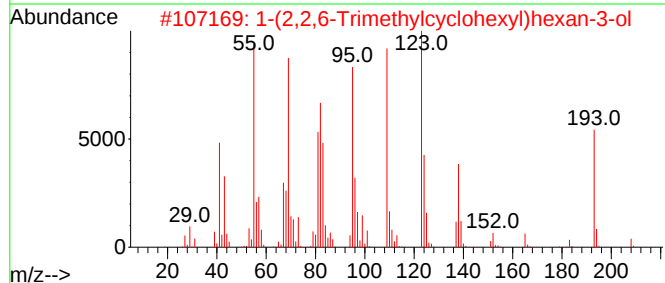
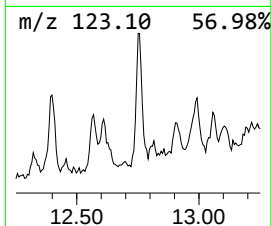
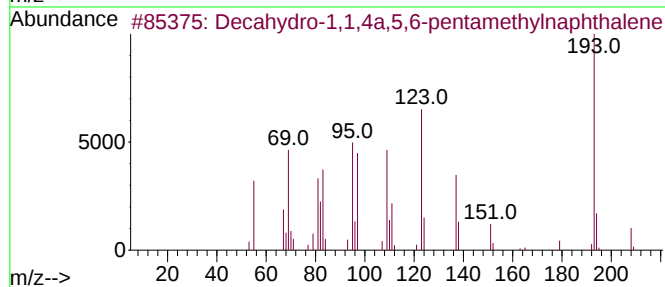
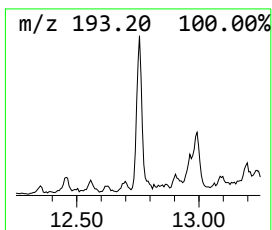
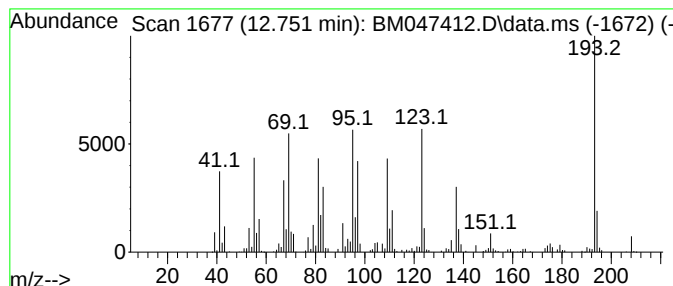
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown12.751 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.751	3.25 ng	397099	Acenaphthene-d10	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	43
2			1-(2,2,6-Trimethylcyclohexyl)hex...	226	C15H30O	070788-30-6	38
3			Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	020536-40-7	35
4			Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	020536-41-8	35
5			Bicyclo[4.1.0]heptane, 3,7,7-tri...	138	C10H18	000554-59-6	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047412.D
Acq On : 30 Aug 2024 18:59
Operator : RC/JU
Sample : P3794-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

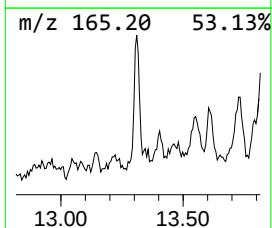
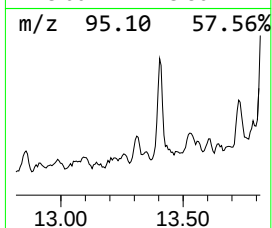
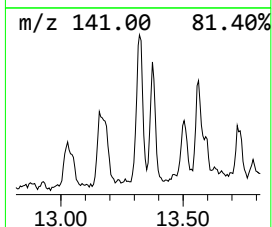
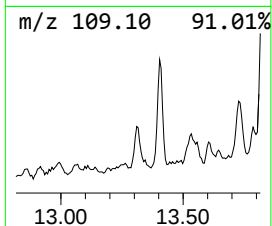
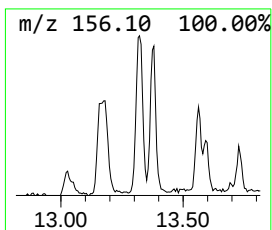
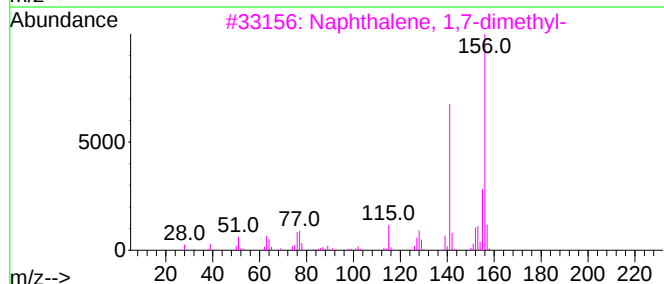
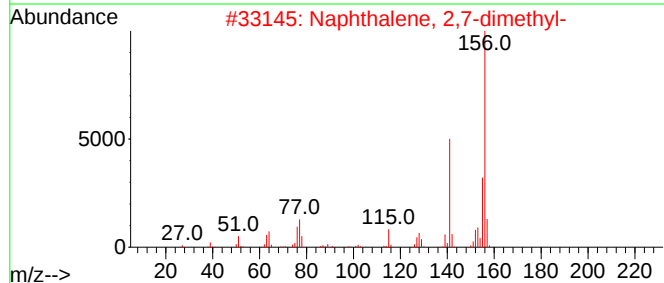
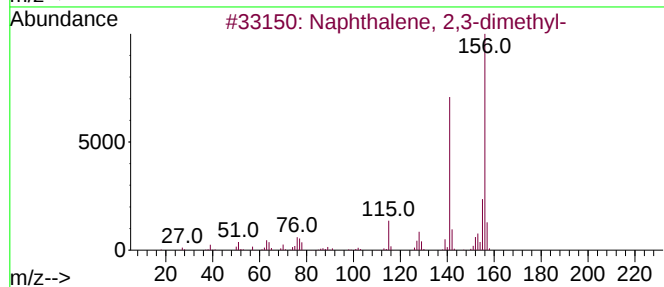
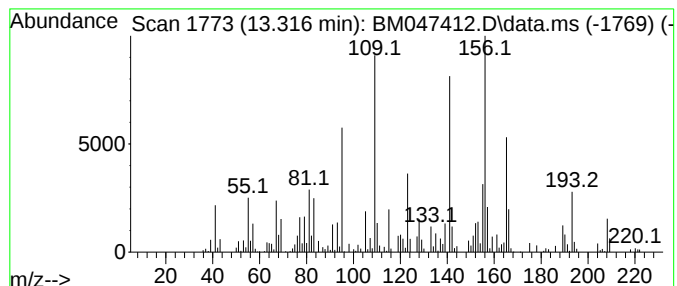
Instrument :
BNA_M
ClientSampleId :
RT-857

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Naphthalene, 2,3-dimethyl- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.316	2.29 ng	279640	Acenaphthene-d10	14.004	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	86
2	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	86
3	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	84
4	Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	83
5	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047412.D
Acq On : 30 Aug 2024 18:59
Operator : RC/JU
Sample : P3794-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RT-857

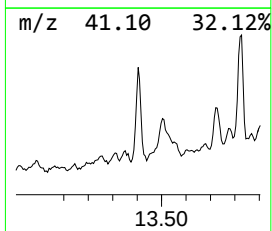
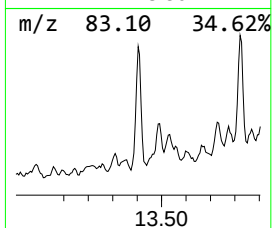
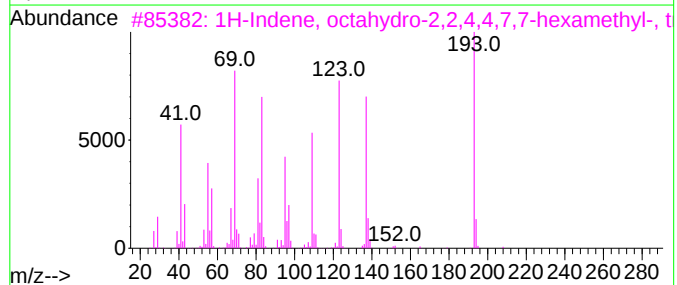
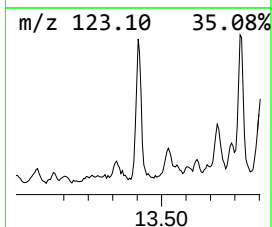
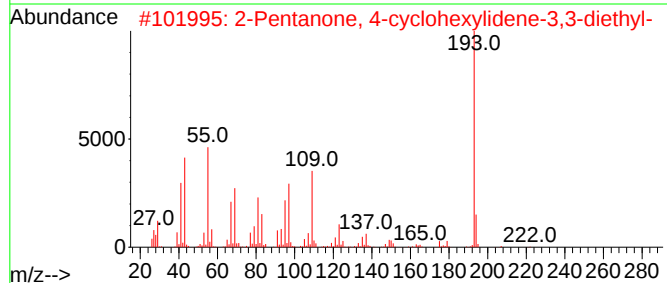
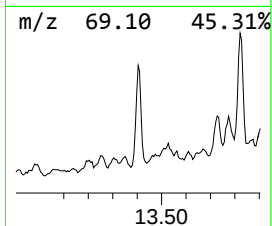
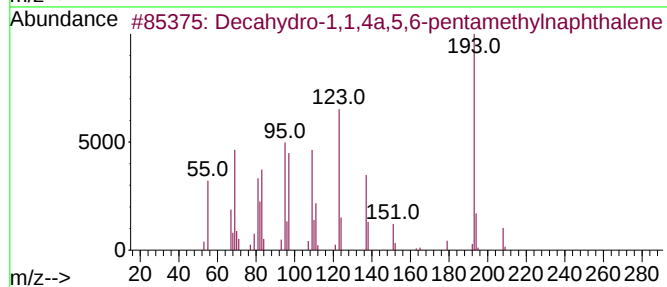
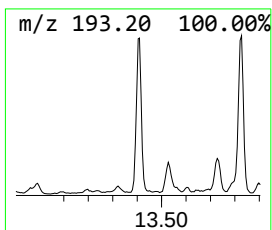
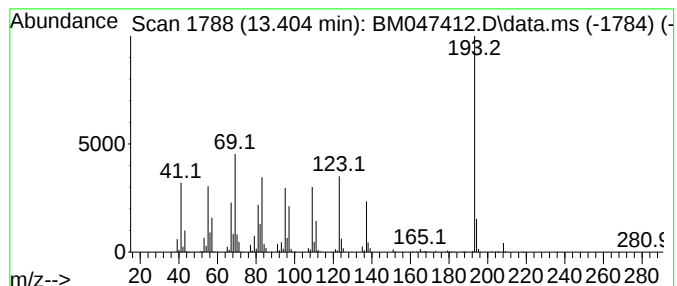
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown13.404 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.404	10.00 ng	1221870	Acenaphthene-d10	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	43
2			2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	42
3			1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	38
4			1-Methyl-3-(trifluoromethyl)-1H...	193	C7H10F3N3	1000511-73-1	38
5			1-Anthracenamine	193	C14H11N	000610-49-1	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047412.D
Acq On : 30 Aug 2024 18:59
Operator : RC/JU
Sample : P3794-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RT-857

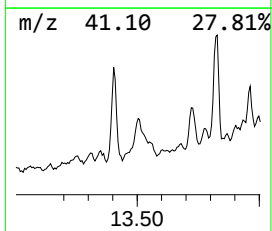
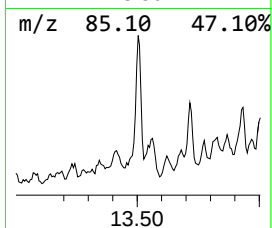
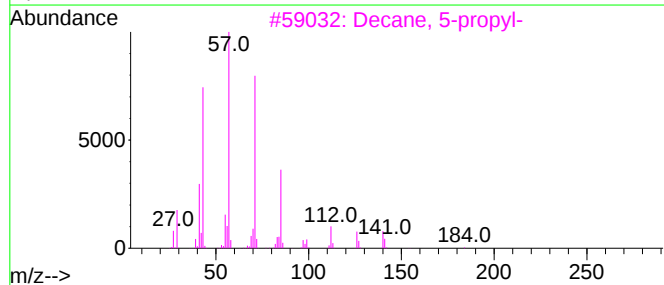
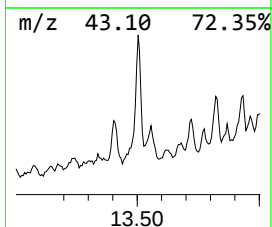
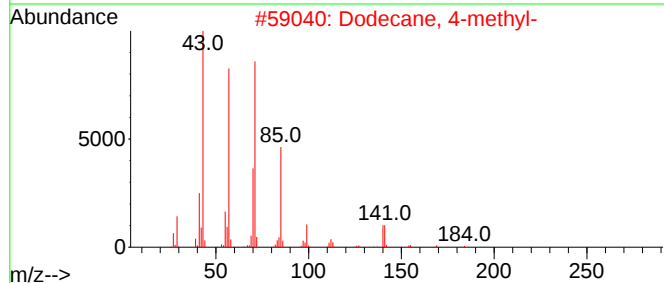
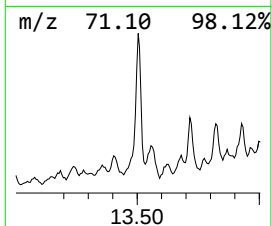
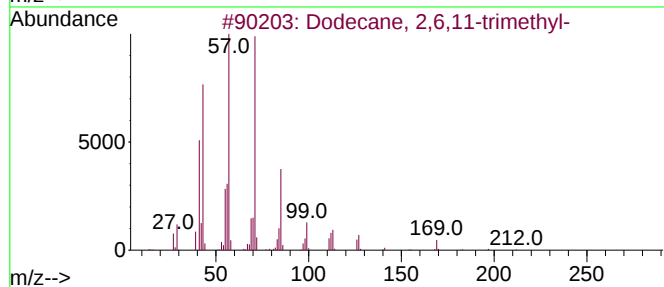
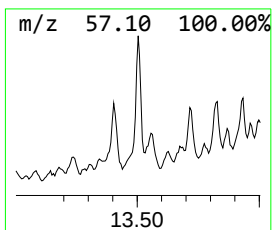
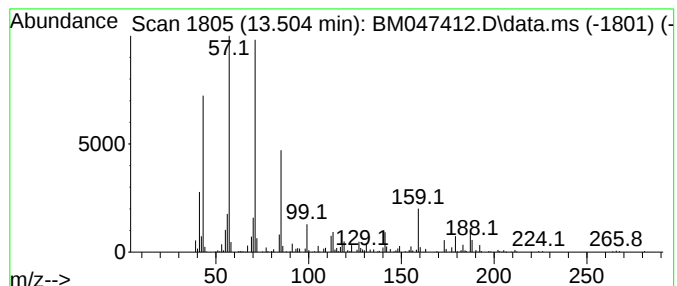
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Dodecane, 2,6,11-trimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.504	5.16 ng	630918	Acenaphthene-d10	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	68
2			Dodecane, 4-methyl-	184	C13H28	006117-97-1	68
3			Decane, 5-propyl-	184	C13H28	017312-62-8	68
4			Decane, 2-methyl-	156	C11H24	006975-98-0	64
5			Hexadecane	226	C16H34	000544-76-3	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047412.D
Acq On : 30 Aug 2024 18:59
Operator : RC/JU
Sample : P3794-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

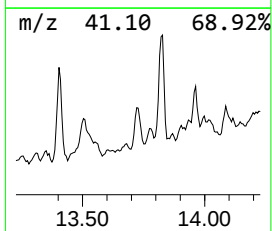
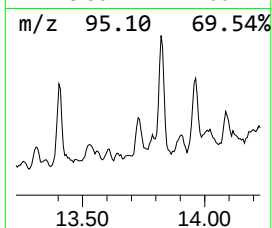
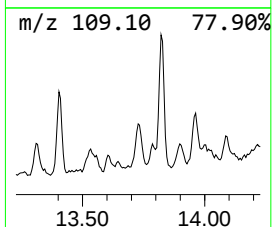
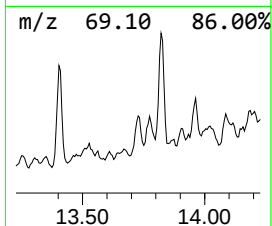
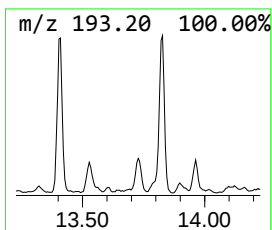
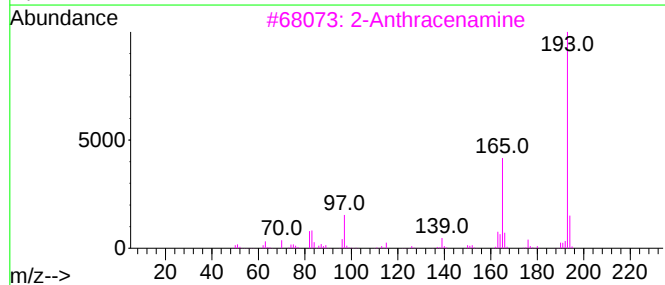
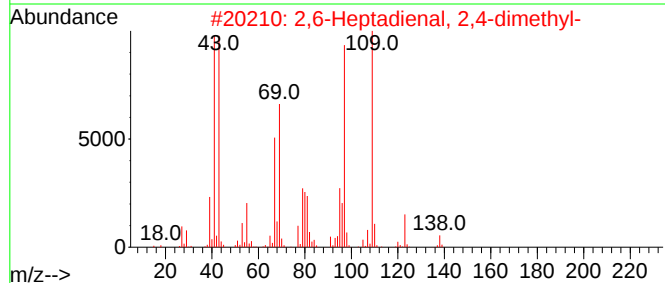
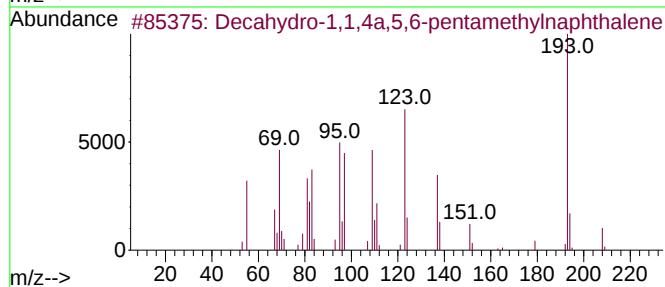
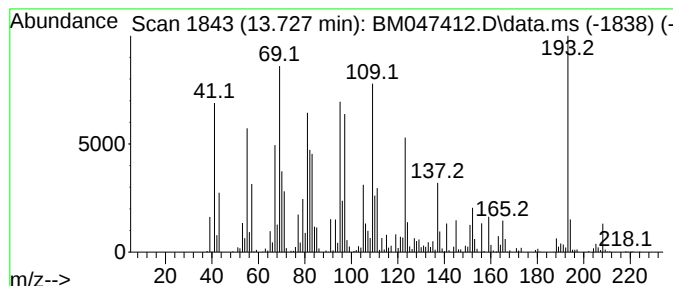
Instrument :
BNA_M
ClientSampleId :
RT-857

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.727	6.96 ng	849822	Acenaphthene-d10	14.004	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	92
2	2,6-Heptadienal, 2,4-dimethyl-	138	C9H14O	085136-08-9	45
3	2-Anthracenamine	193	C14H11N	000613-13-8	35
4	1-Anthracenamine	193	C14H11N	000610-49-1	35
5	Oxiranecarboxaldehyde, 3-methyl-...	168	C10H16O2	016996-12-6	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047412.D
Acq On : 30 Aug 2024 18:59
Operator : RC/JU
Sample : P3794-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RT-857

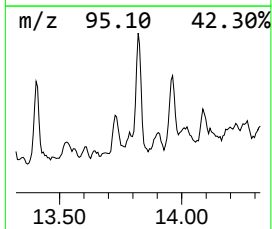
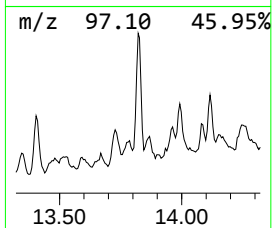
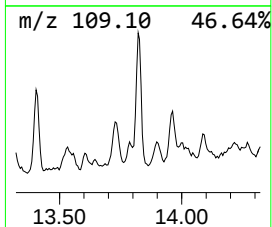
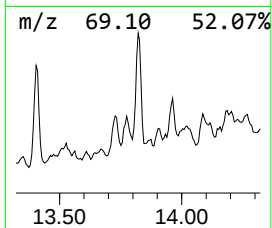
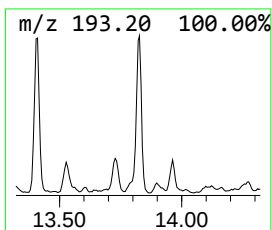
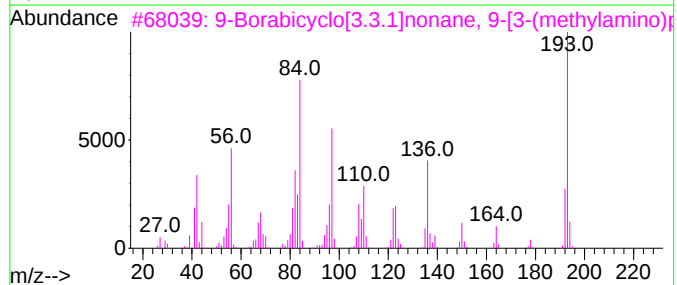
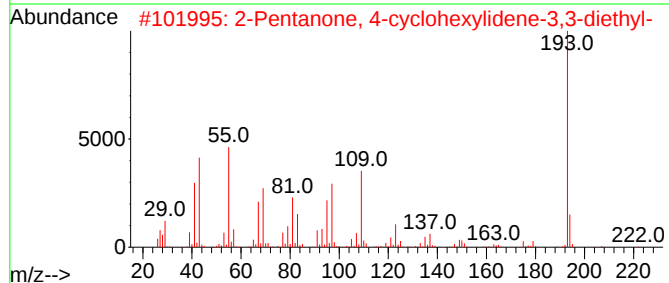
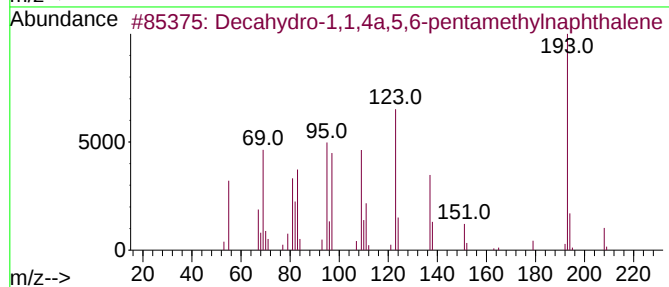
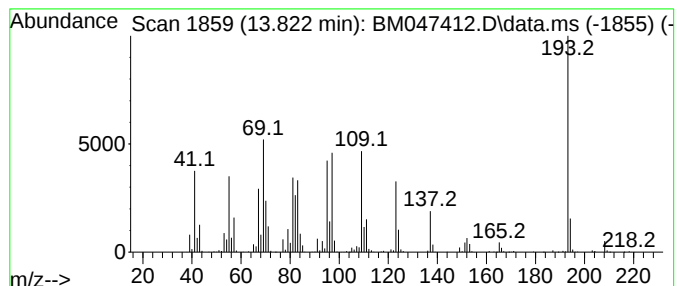
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 unknown13.822 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.822	12.78 ng	1561710	Acenaphthene-d10	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	49
2			2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	45
3			9-Borabicyclo[3.3.1]nonane, 9-[3...	193	C12H24BN	1010162-56-0	43
4			1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	38
5			Borinic acid, diethyl-, 3,3,5-tr...	208	C13H25BO	057387-76-5	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047412.D
Acq On : 30 Aug 2024 18:59
Operator : RC/JU
Sample : P3794-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

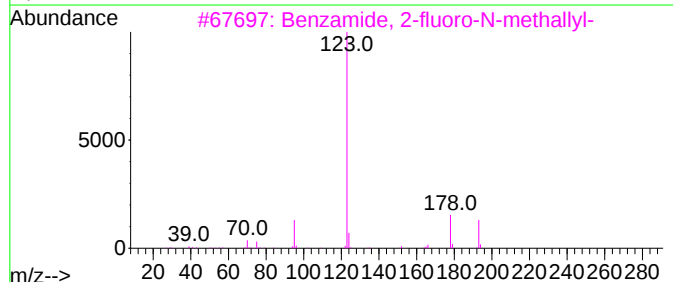
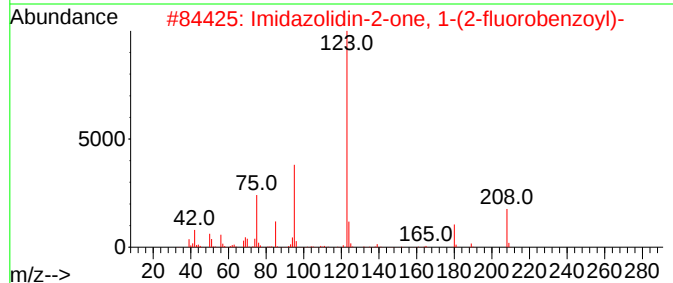
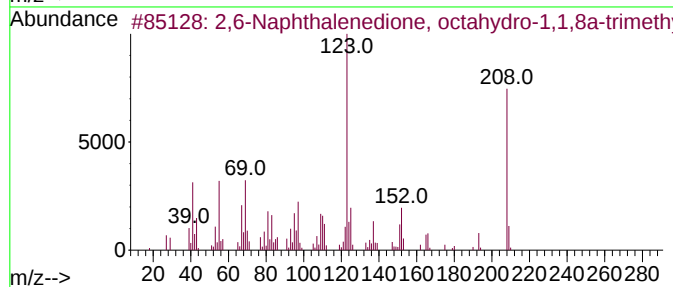
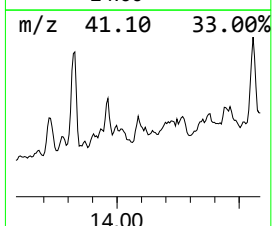
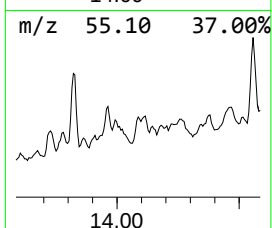
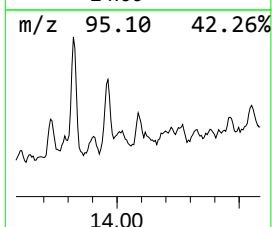
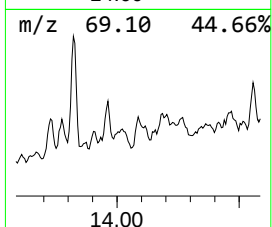
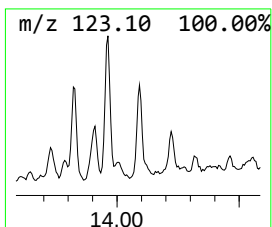
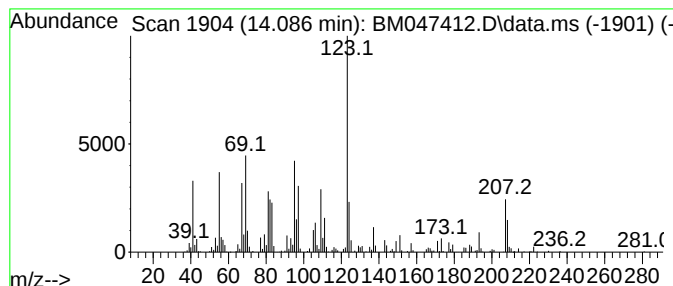
Instrument :
BNA_M
ClientSampleId :
RT-857

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 2,6-Naphthalenedione, octah... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.086	4.04 ng	493768	Acenaphthene-d10		14.004	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2,6-Naphthalenedione, octahydro-...		208	C13H20O2	057289-17-5	68
2	Imidazolidin-2-one, 1-(2-fluorob...		208	C10H9FN2O2	1010310-62-2	46
3	Benzamide, 2-fluoro-N-methallyl-		193	C11H12FNO	1000340-07-0	43
4	1-(4-Fluorobenzoyl)piperazine		208	C11H13FN2O	102391-98-0	43
5	Benzamide, 3-fluoro-N-(2-phenyle...		299	C19H22FNO	1000451-30-2	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047412.D
Acq On : 30 Aug 2024 18:59
Operator : RC/JU
Sample : P3794-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

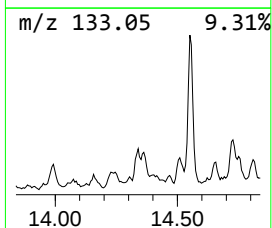
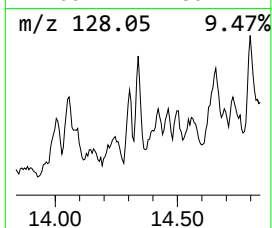
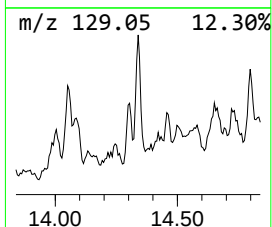
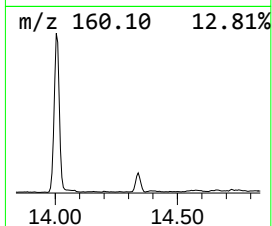
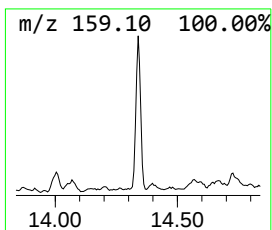
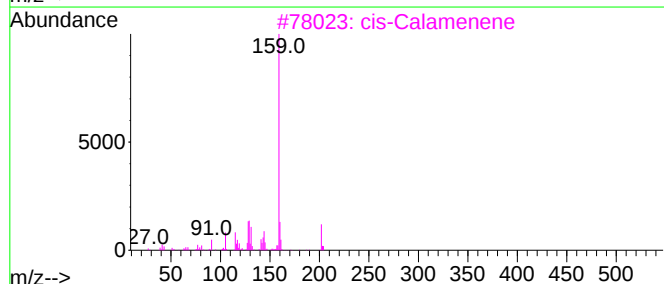
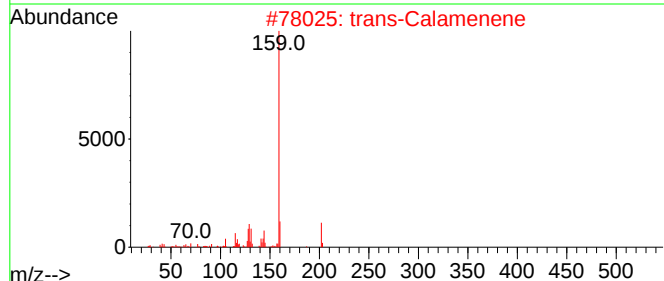
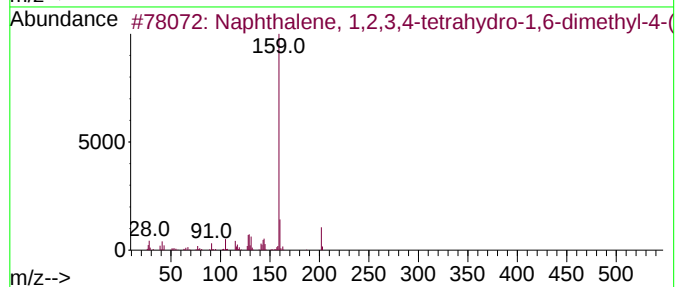
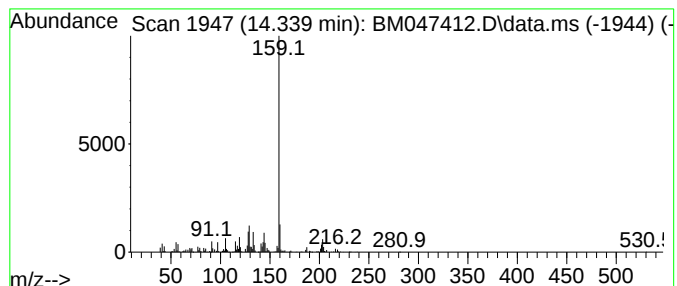
Instrument :
BNA_M
ClientSampleId :
RT-857

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.339	4.02 ng	491070	Acenaphthene-d10	14.004	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	202	C15H22	000483-77-2	91
2	trans-Calamenene	202	C15H22	073209-42-4	91
3	cis-Calamenene	202	C15H22	072937-55-4	91
4	2-Phenylpropionic acid, 4'-(2-me...	218	C14H18O2	1010454-94-3	76
5	Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	000475-03-6	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047412.D
Acq On : 30 Aug 2024 18:59
Operator : RC/JU
Sample : P3794-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RT-857

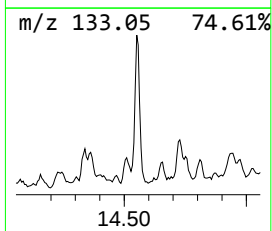
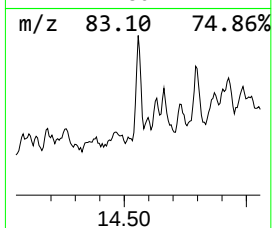
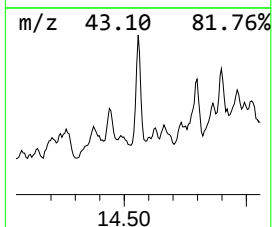
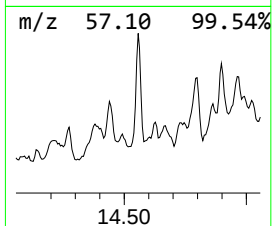
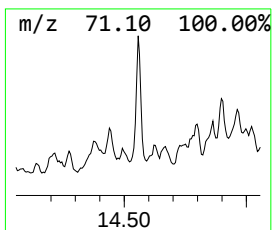
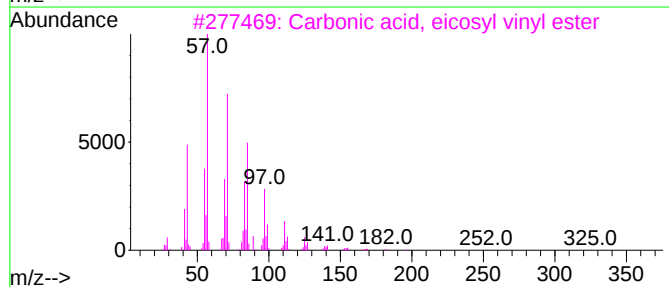
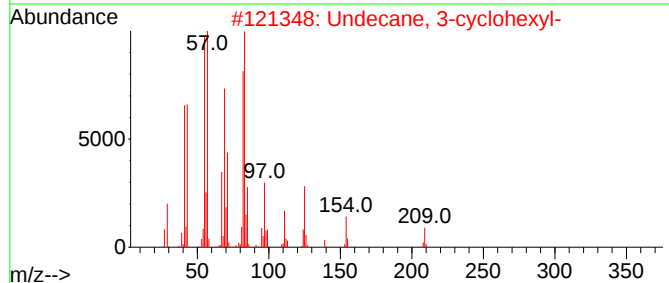
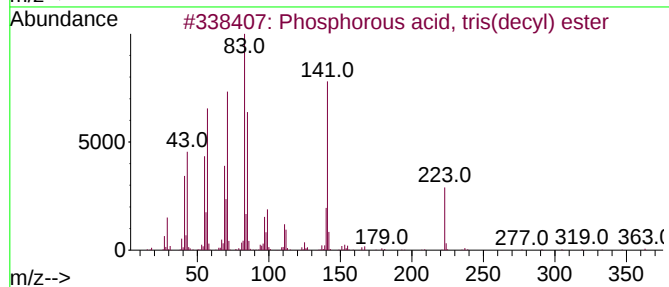
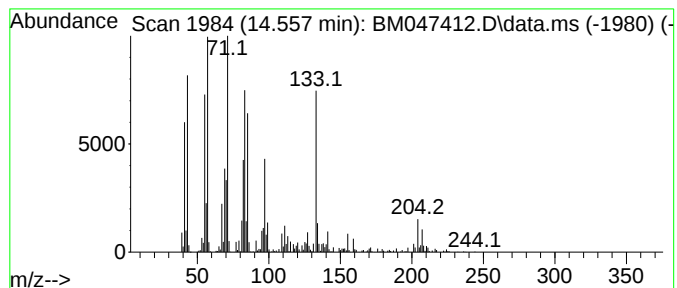
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 unknown14.557 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.557	11.05 ng	1349330	Acenaphthene-d10	14.004

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Phosphorous acid, tris(decyl) ester	502	C30H63O3P	002929-86-4	45
2		Undecane, 3-cyclohexyl-	238	C17H34	013151-78-5	38
3		Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	38
4		Decane, 3,7-dimethyl-	170	C12H26	017312-54-8	35
5		Dodecane, 4-methyl-	184	C13H28	006117-97-1	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047412.D
Acq On : 30 Aug 2024 18:59
Operator : RC/JU
Sample : P3794-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RT-857

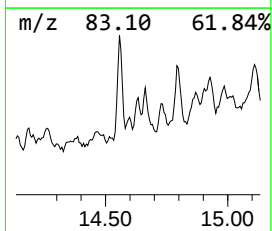
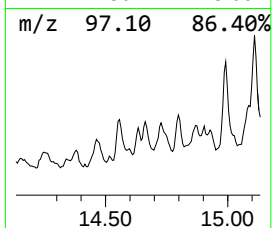
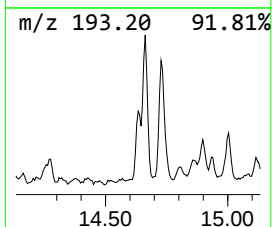
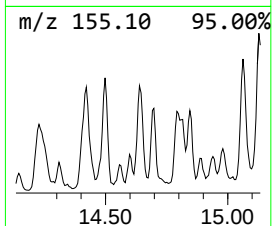
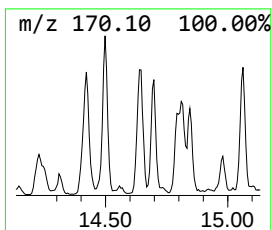
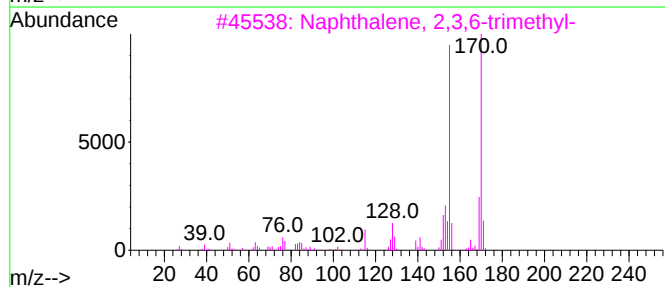
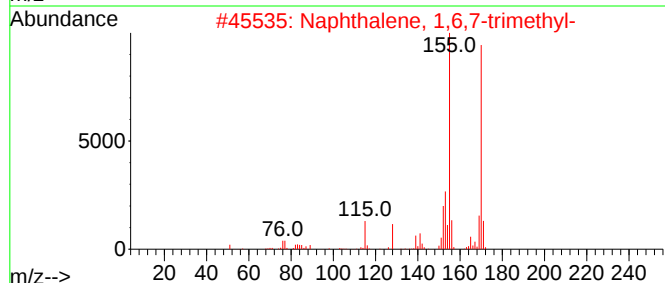
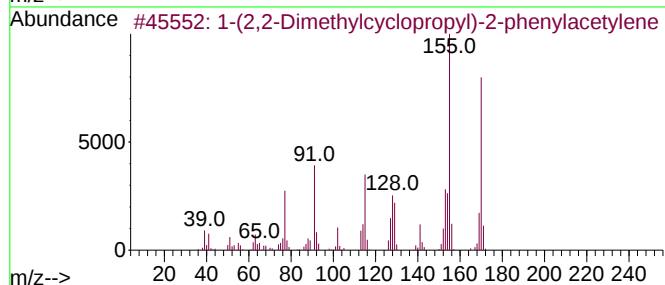
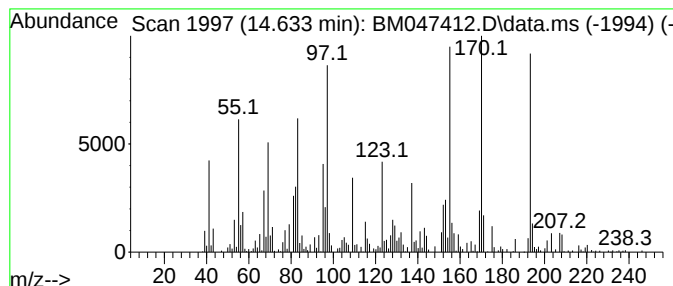
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 1-(2,2-Dimethylcyclopropyl)... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.633	2.96 ng	361198	Acenaphthene-d10	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(2,2-Dimethylcyclopropyl)-2-ph...		170	C13H14		1000294-91-1	84
2	Naphthalene, 1,6,7-trimethyl-		170	C13H14		002245-38-7	84
3	Naphthalene, 2,3,6-trimethyl-		170	C13H14		000829-26-5	81
4	4,6,8-Trimethylazulene		170	C13H14		000941-81-1	59
5	Naphthalene, 1,4,5-trimethyl-		170	C13H14		002131-41-1	56



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047412.D
Acq On : 30 Aug 2024 18:59
Operator : RC/JU
Sample : P3794-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RT-857

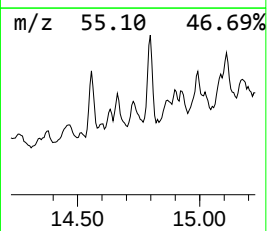
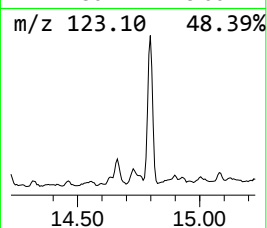
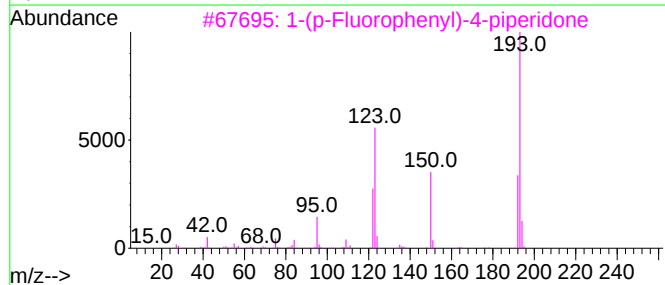
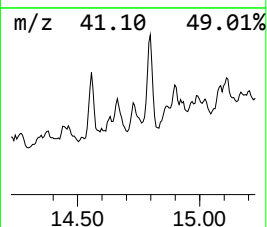
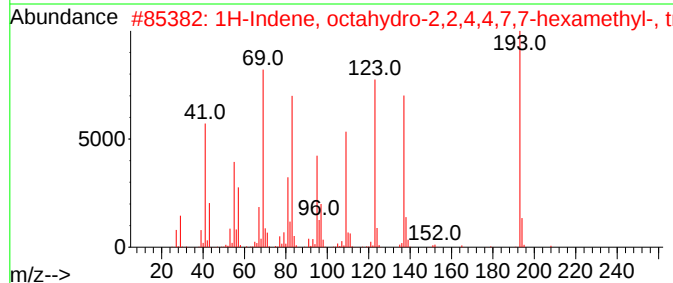
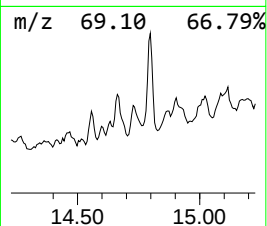
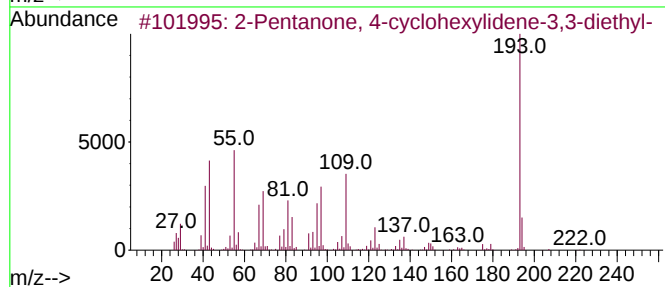
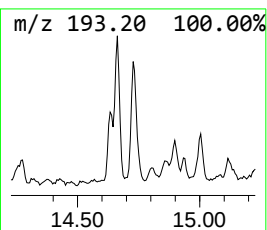
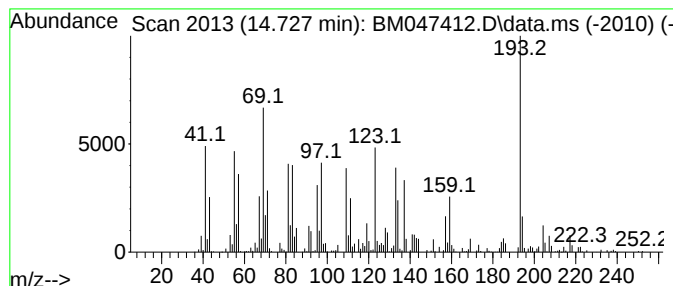
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 unknown14.727 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.727	6.34 ng	774697	Acenaphthene-d10	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	43		
2	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	37		
3	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	30		
4	2-Anthracenamine	193	C14H11N	000613-13-8	27		
5	Butan-2-one, 1-[3-(3,3-dimethyl-...	278	C16H26N2O2	1000303-34-2	22		



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047412.D
Acq On : 30 Aug 2024 18:59
Operator : RC/JU
Sample : P3794-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RT-857

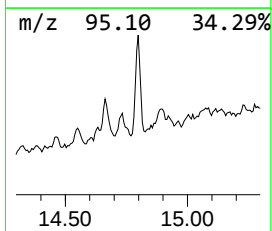
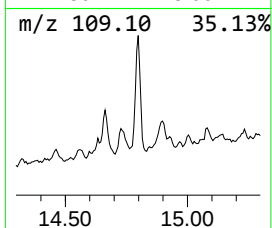
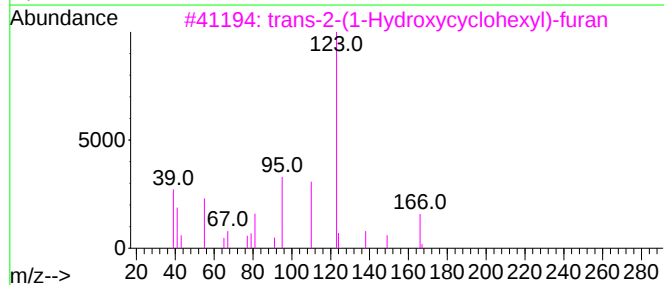
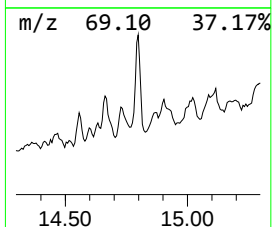
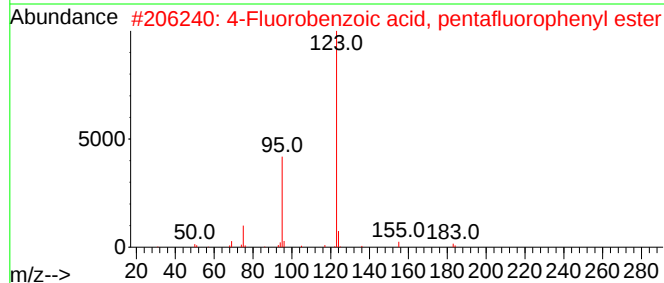
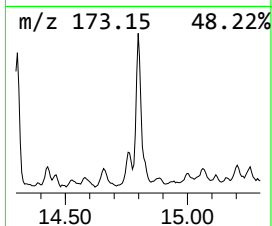
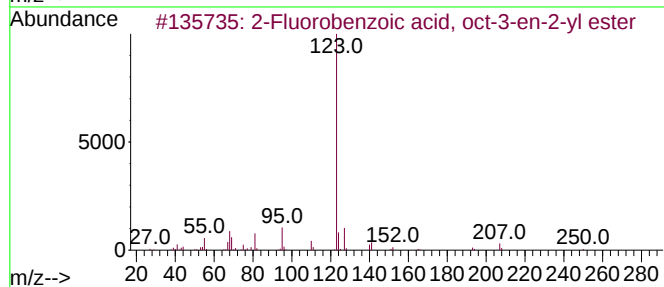
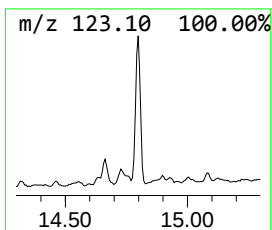
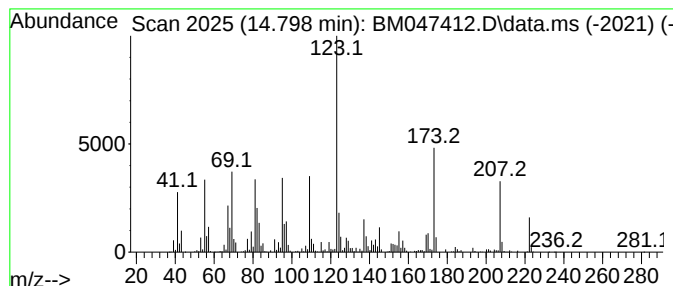
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 unknown14.798 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.798	19.11 ng	2334550	Acenaphthene-d10	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Fluorobenzoic acid, oct-3-en-2...	250	C15H19F02	1000299-16-5	37		
2	4-Fluorobenzoic acid, pentafluor...	306	C13H4F6O2	1000355-67-4	35		
3	trans-2-(1-Hydroxycyclohexyl)-furan	166	C10H14O2	115754-87-5	35		
4	5-Fluoroisobenzofuran-1(3H)-one	152	C8H5F02	000700-85-6	35		
5	1-Butanone, 1-bicyclo[4.1.0]hept...	166	C11H18O	054764-62-4	35		



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047412.D
Acq On : 30 Aug 2024 18:59
Operator : RC/JU
Sample : P3794-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RT-857

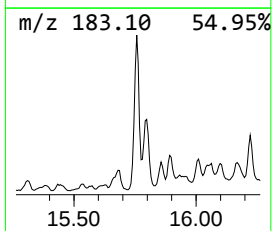
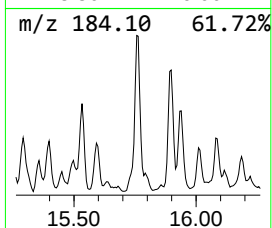
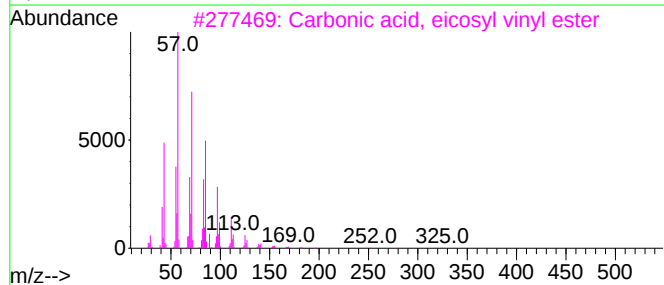
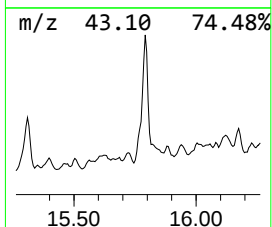
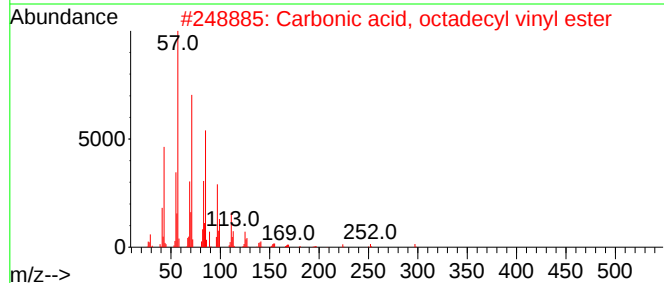
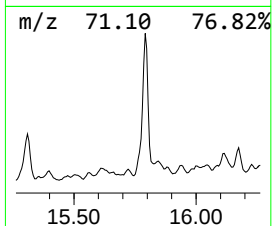
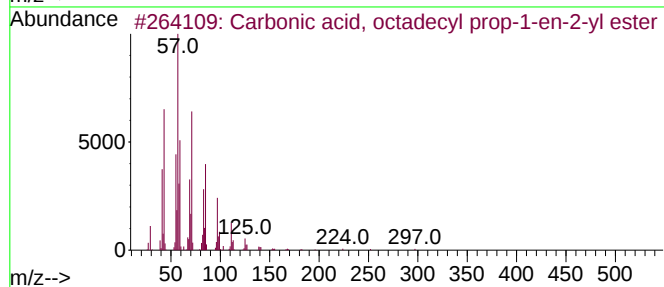
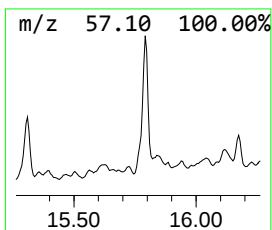
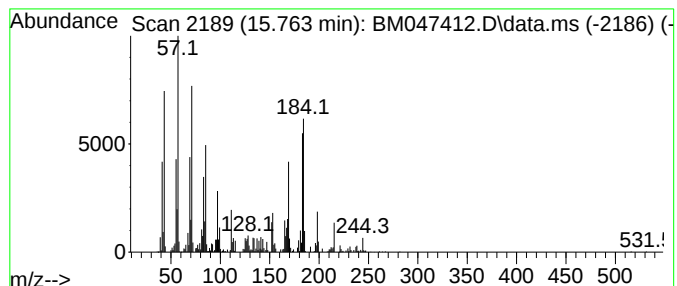
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 Carbonic acid, octadecyl pr... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.763	15.33 ng	1203740	Phenanthrene-d10	16.780

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	50
2			Carbonic acid, octadecyl vinyl e...	340	C21H40O3	1000382-54-4	50
3			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	50
4			Tetradecane	198	C14H30	000629-59-4	46
5			Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047412.D
Acq On : 30 Aug 2024 18:59
Operator : RC/JU
Sample : P3794-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

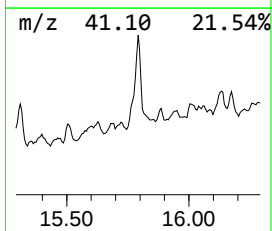
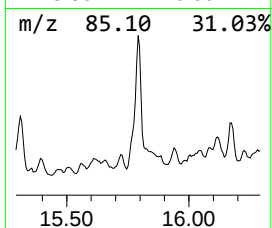
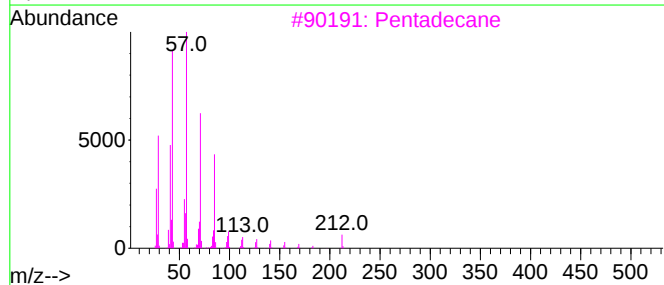
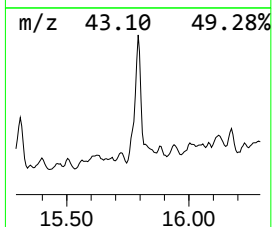
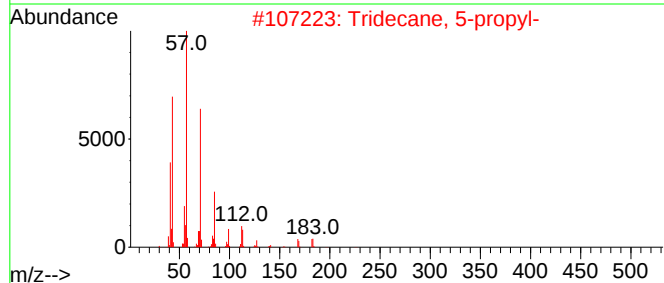
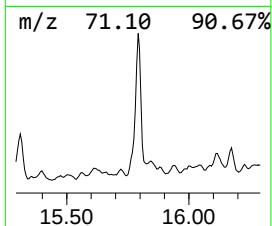
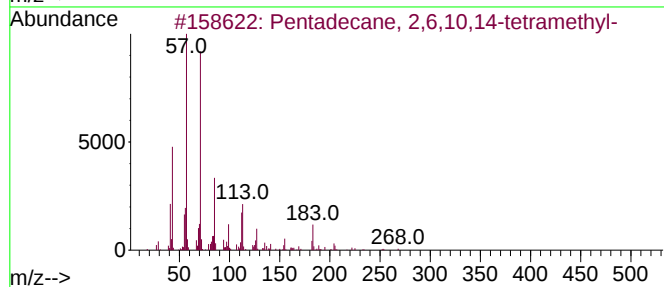
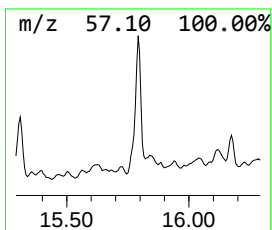
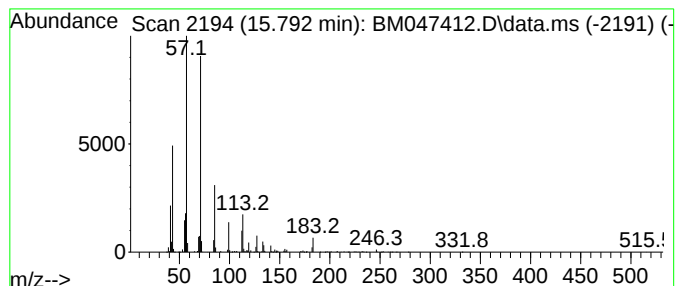
Instrument :
BNA_M
ClientSampleId :
RT-857

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 Pentadecane, 2,6,10,14-tetr... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
15.792	38.86 ng	3051120	Phenanthrene-d10		16.780	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	91
2		Tridecane, 5-propyl-	226	C16H34	055045-11-9	68
3		Pentadecane	212	C15H32	000629-62-9	64
4		Bacchotricuneatin c	342	C20H22O5	066563-30-2	59
5		Dodecane	170	C12H26	000112-40-3	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047412.D
Acq On : 30 Aug 2024 18:59
Operator : RC/JU
Sample : P3794-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

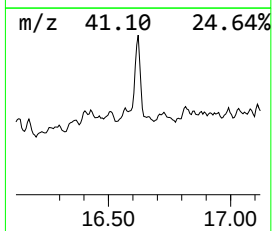
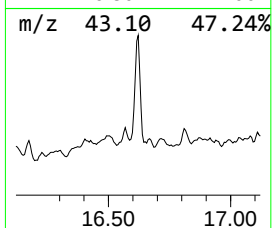
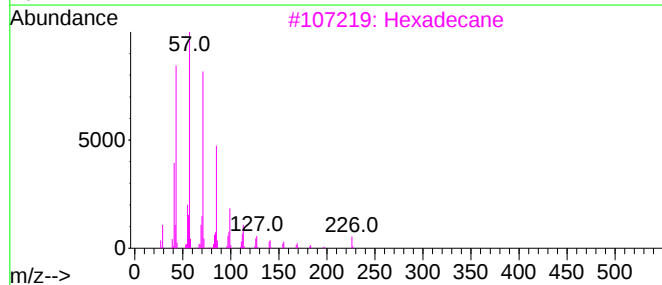
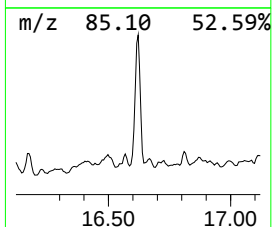
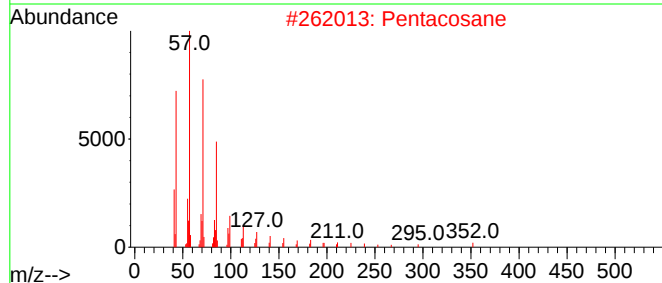
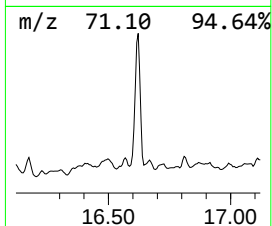
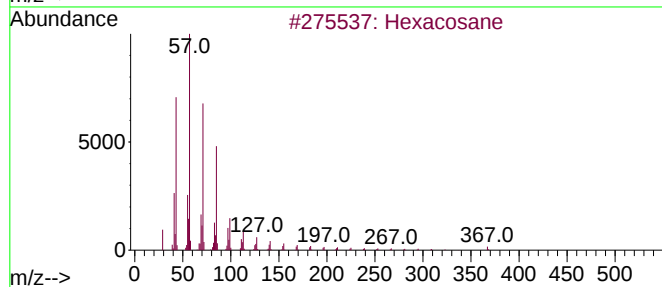
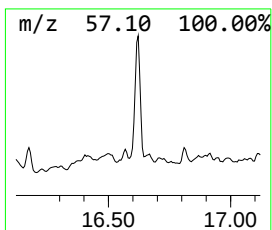
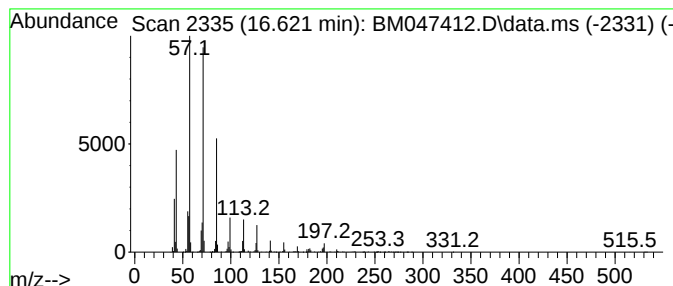
Instrument :
BNA_M
ClientSampleId :
RT-857

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 17 Hexacosane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
16.621	66.16 ng	5194120	Phenanthrene-d10		16.780	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Hexacosane		366	C26H54	000630-01-3	90
2	Pentacosane		352	C25H52	000629-99-2	90
3	Hexadecane		226	C16H34	000544-76-3	86
4	2-Bromotetradecane		276	C14H29Br	074036-95-6	86
5	Pentadecane, 4-methyl-		226	C16H34	002801-87-8	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
Data File : BM047412.D
Acq On : 30 Aug 2024 18:59
Operator : RC/JU
Sample : P3794-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RT-857

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.557	3.5	ng	224100	1	7.345	1281170	20.0
1-Phenoxypropan...	10.869	2.0	ng	166482	2	10.098	1660930	20.0
unknown12.751	12.751	3.3	ng	397099	3	14.004	2443230	20.0
Naphthalene, 2,...	13.316	2.3	ng	279640	3	14.004	2443230	20.0
unknown13.404	13.404	10.0	ng	1221870	3	14.004	2443230	20.0
Dodecane, 2,6,1...	13.504	5.2	ng	630918	3	14.004	2443230	20.0
Decahydro-1,1,4...	13.727	7.0	ng	849822	3	14.004	2443230	20.0
unknown13.822	13.822	12.8	ng	1561710	3	14.004	2443230	20.0
2,6-Naphthalene...	14.086	4.0	ng	493768	3	14.004	2443230	20.0
Naphthalene, 1,...	14.339	4.0	ng	491070	3	14.004	2443230	20.0
unknown14.557	14.557	11.1	ng	1349330	3	14.004	2443230	20.0
1-(2,2-Dimethyl...	14.633	3.0	ng	361198	3	14.004	2443230	20.0
unknown14.727	14.727	6.3	ng	774697	3	14.004	2443230	20.0
unknown14.798	14.798	19.1	ng	2334550	3	14.004	2443230	20.0
Carbonic acid, ...	15.763	15.3	ng	1203740	4	16.780	1570140	20.0
Pentadecane, 2,...	15.792	38.9	ng	3051120	4	16.780	1570140	20.0
Hexacosane	16.621	66.2	ng	5194120	4	16.780	1570140	20.0