

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
 Data File : BF139092.D
 Acq On : 21 Aug 2024 10:22
 Operator : RC/JU
 Sample : P3663-08
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 916-J-SD-0.5-1-081624

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_F\Methods\8270-BF082024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139092.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.193	10	17	24	rBV	1206024	1851815	100.00%	11.911%
2	3.393	213	221	233	rBV	28894	76975	4.16%	0.495%
3	3.987	317	322	329	rVB	14187	21831	1.18%	0.140%
4	5.110	504	513	520	rBV	69912	112088	6.05%	0.721%
5	5.510	575	581	586	rBV	1221283	1590377	85.88%	10.229%
6	6.510	745	751	757	rVV	1207538	1632059	88.13%	10.497%
7	6.716	781	786	792	rBV	24503	31432	1.70%	0.202%
8	6.892	811	816	822	rBV	423774	545955	29.48%	3.512%
9	7.051	833	843	848	rBV	156206	195691	10.57%	1.259%
10	7.451	905	911	916	rBV	759227	993888	53.67%	6.393%
11	8.175	1029	1034	1040	rBV	562997	703245	37.98%	4.523%
12	8.486	1083	1087	1095	rBV	40446	53646	2.90%	0.345%
13	9.251	1211	1217	1222	rBV	1136060	1373297	74.16%	8.833%
14	9.933	1327	1333	1343	rVB	633669	810412	43.76%	5.212%
15	10.027	1343	1349	1356	rBV2	41293	75666	4.09%	0.487%
16	10.651	1448	1455	1459	rBV5	9115	20333	1.10%	0.131%
17	10.716	1460	1466	1471	rVV	786055	989288	53.42%	6.363%
18	10.839	1483	1487	1496	rVB2	16931	23609	1.27%	0.152%
19	11.416	1574	1585	1590	rBV	623719	791458	42.74%	5.091%
20	11.533	1599	1605	1610	rBV4	51372	79960	4.32%	0.514%
21	11.851	1655	1659	1668	rVB	71301	113504	6.13%	0.730%
22	11.945	1668	1675	1684	rBV2	202248	354802	19.16%	2.282%
23	12.010	1684	1686	1693	rVB3	14005	20653	1.12%	0.133%
24	12.733	1803	1809	1819	rVB	106050	164114	8.86%	1.056%
25	12.957	1842	1847	1850	rBV	17454	23527	1.27%	0.151%
26	13.004	1850	1855	1860	rVB	671093	851255	45.97%	5.475%
27	13.474	1927	1935	1942	rBV5	9024	22326	1.21%	0.144%
28	13.580	1946	1953	1961	rVB9	6491	20117	1.09%	0.129%
29	13.904	2003	2008	2021	rBV	115425	192183	10.38%	1.236%
30	14.051	2028	2033	2039	rVB	318124	399101	21.55%	2.567%
31	14.545	2111	2117	2129	rBV	123931	211317	11.41%	1.359%
32	14.751	2147	2152	2159	rBV2	16377	26493	1.43%	0.170%
33	15.198	2223	2228	2230	rBV	24118	36429	1.97%	0.234%
34	15.227	2230	2233	2239	rVB2	31964	52505	2.84%	0.338%
35	15.480	2270	2276	2279	rBV5	16875	32700	1.77%	0.210%
36	15.533	2279	2285	2291	rVB	320793	488935	26.40%	3.145%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
Data File : BF139092.D
Acq On : 21 Aug 2024 10:22
Operator : RC/JU
Sample : P3663-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
916-J-SD-0.5-1-081624

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_F\Methods\8270-BF082024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.792	2326	2329	2338	rVB6	10292	20190	1.09%	0.130%
38	16.039	2366	2371	2375	rBV	17600	29280	1.58%	0.188%
39	16.092	2375	2380	2387	rVB3	23218	45608	2.46%	0.293%
40	16.862	2507	2511	2518	rVB6	9767	19309	1.04%	0.124%
41	17.039	2533	2541	2557	rVB6	33078	102513	5.54%	0.659%
42	17.374	2592	2598	2611	rVB9	16555	49156	2.65%	0.316%
43	17.645	2635	2644	2650	rBV6	23397	61174	3.30%	0.393%
44	17.727	2651	2658	2671	rVB9	31135	94827	5.12%	0.610%
45	17.980	2694	2701	2718	rVB6	37995	119698	6.46%	0.770%
46	18.692	2816	2822	2828	rBV7	8828	22842	1.23%	0.147%

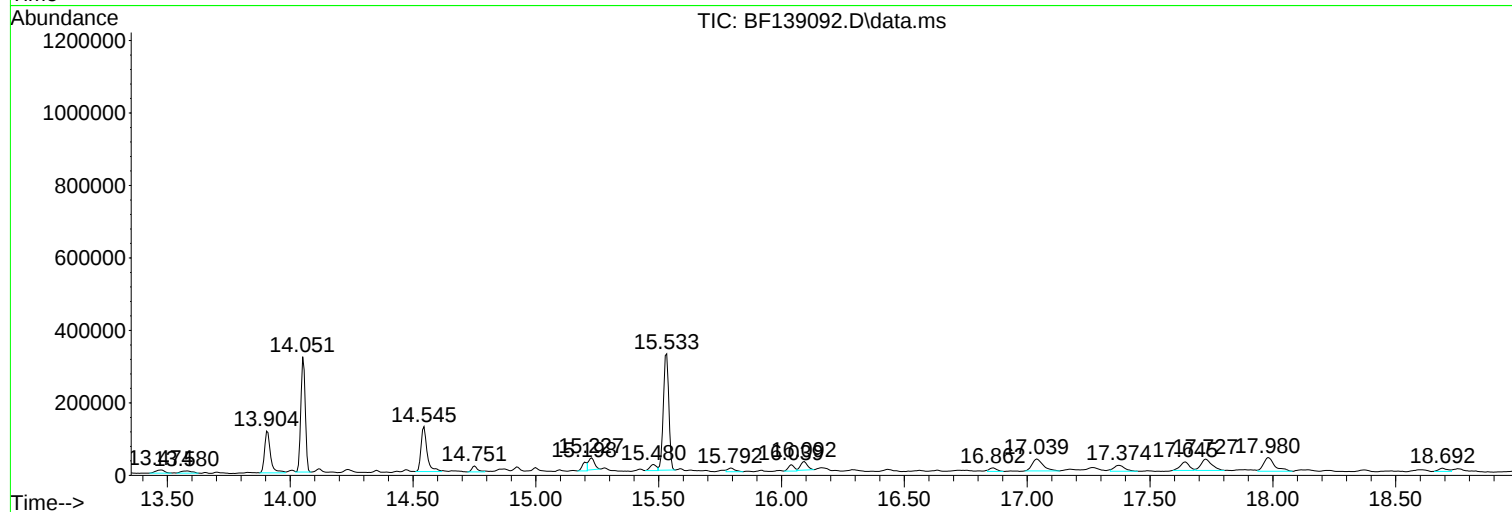
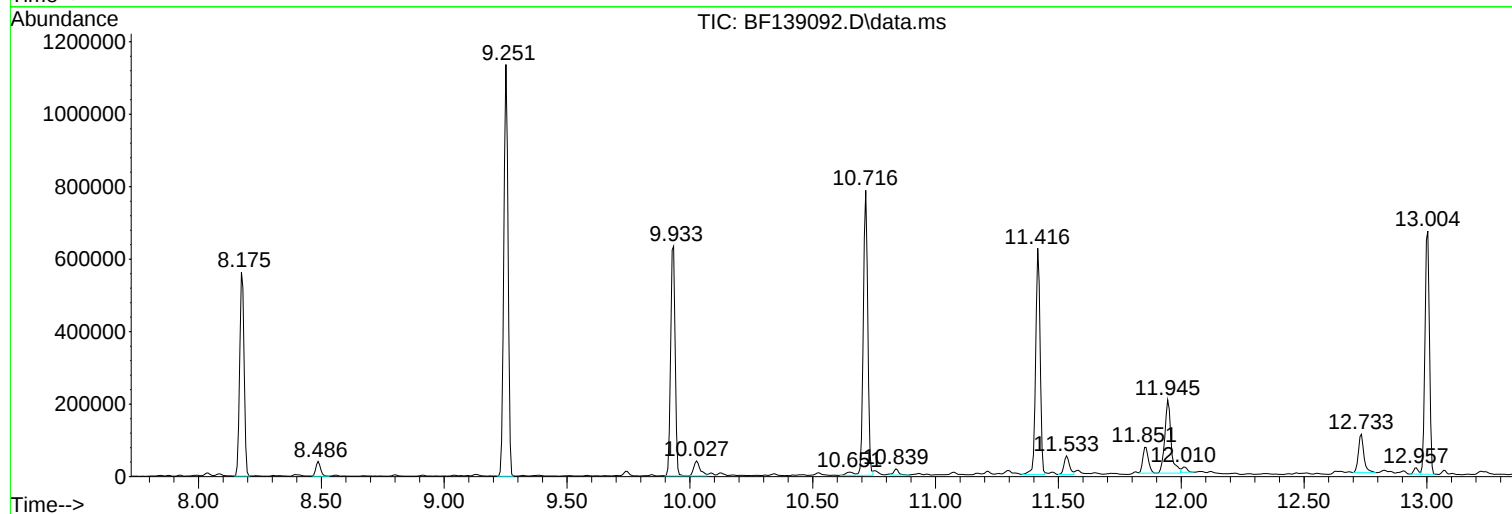
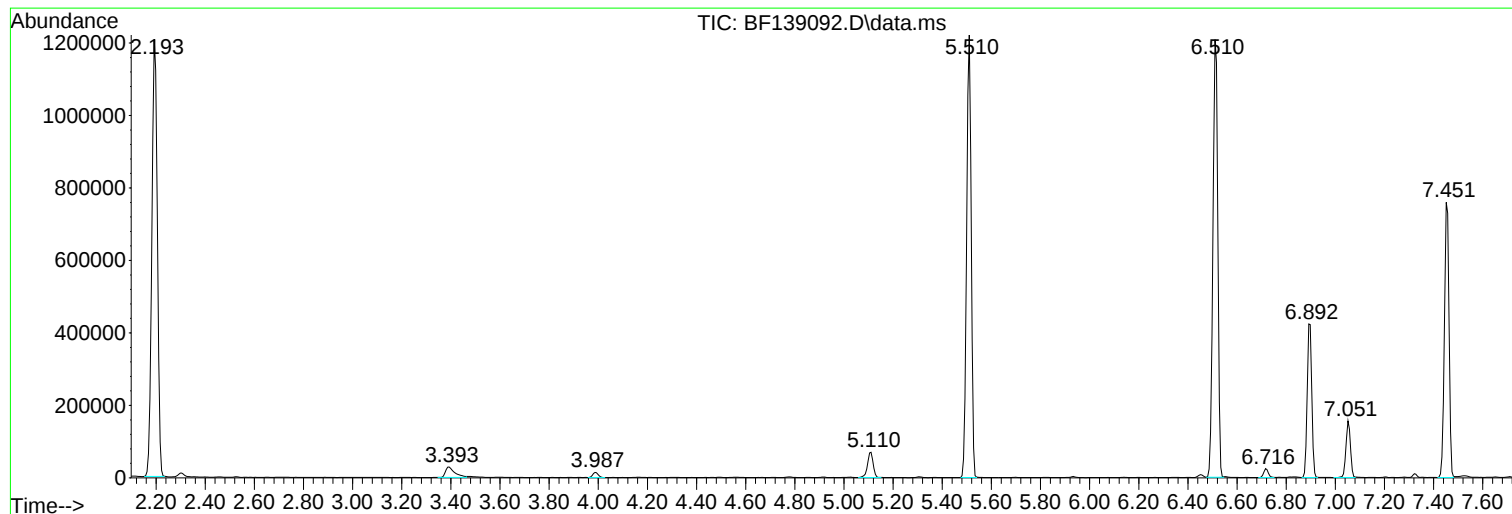
Sum of corrected areas: 15547583

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
Data File : BF139092.D
Acq On : 21 Aug 2024 10:22
Operator : RC/JU
Sample : P3663-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
916-J-SD-0.5-1-081624

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.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_F\Data\BF082124\
Data File : BF139092.D
Acq On : 21 Aug 2024 10:22
Operator : RC/JU
Sample : P3663-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
916-J-SD-0.5-1-081624

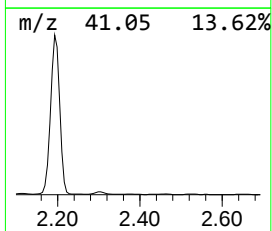
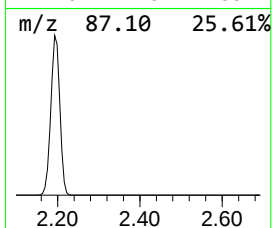
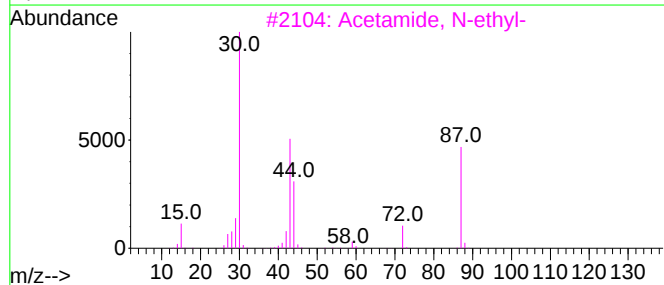
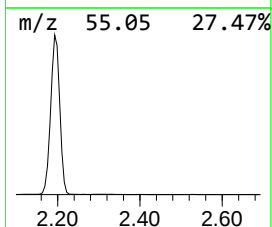
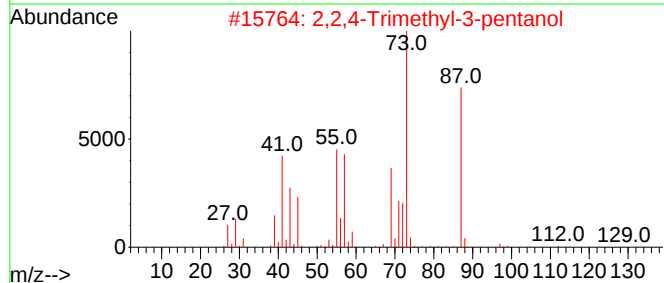
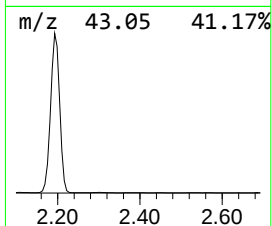
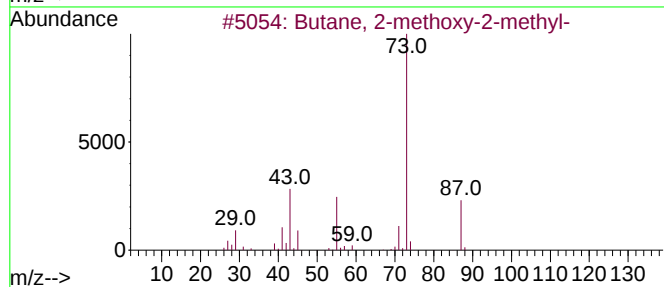
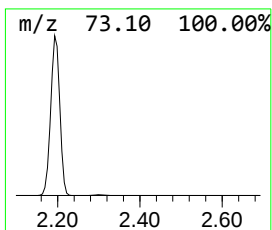
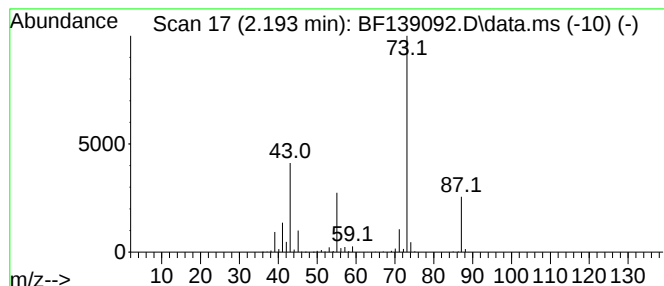
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.193	67.84 ng	1851820	1,4-Dichlorobenzene-d4	6.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
Data File : BF139092.D
Acq On : 21 Aug 2024 10:22
Operator : RC/JU
Sample : P3663-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
916-J-SD-0.5-1-081624

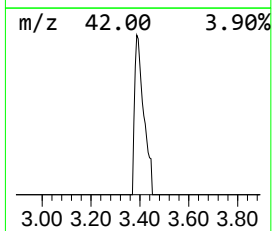
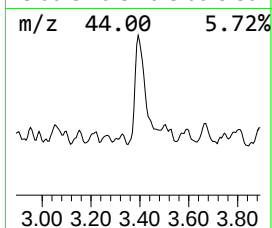
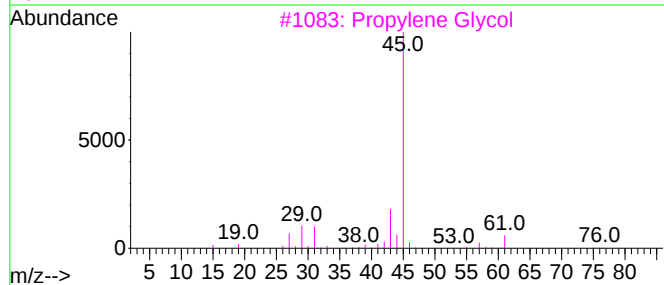
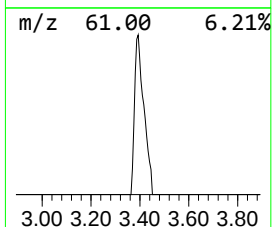
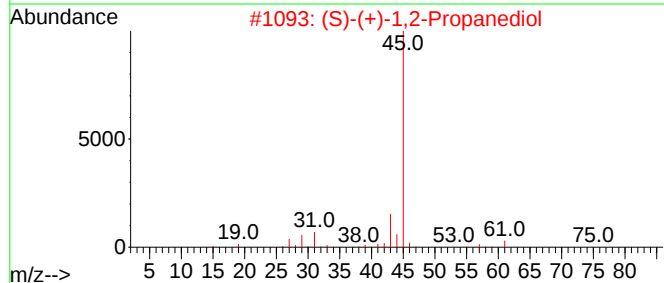
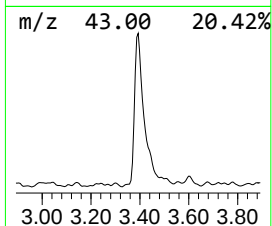
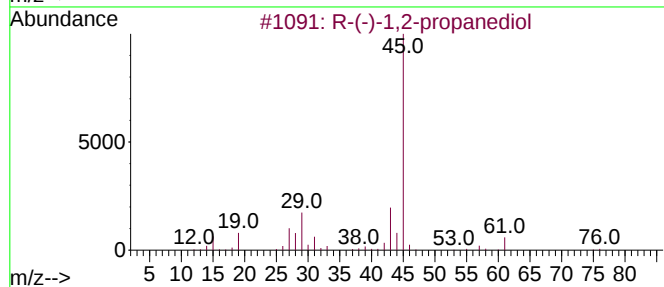
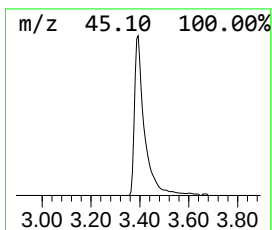
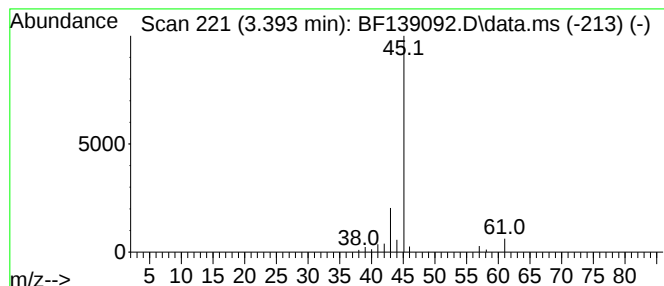
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 R-(-)-1,2-propanediol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.393	2.82 ng	76975	1,4-Dichlorobenzene-d4	6.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	64
2			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
3			Propylene Glycol	76	C3H8O2	000057-55-6	9
4			Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5			Formamide	45	CH3NO	000075-12-7	5



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
Data File : BF139092.D
Acq On : 21 Aug 2024 10:22
Operator : RC/JU
Sample : P3663-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
916-J-SD-0.5-1-081624

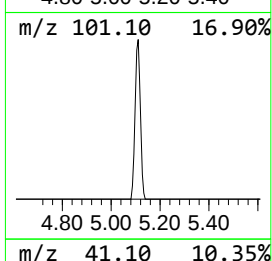
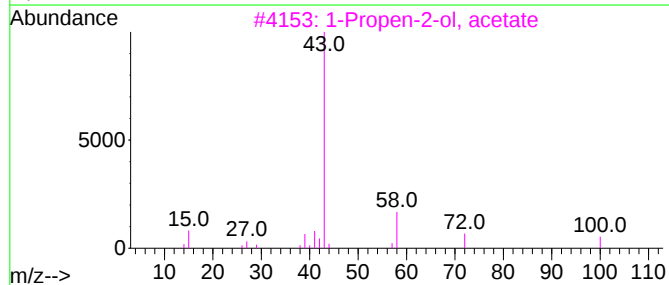
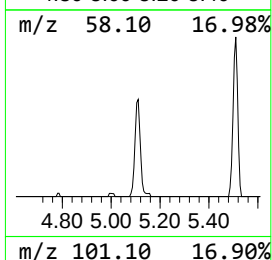
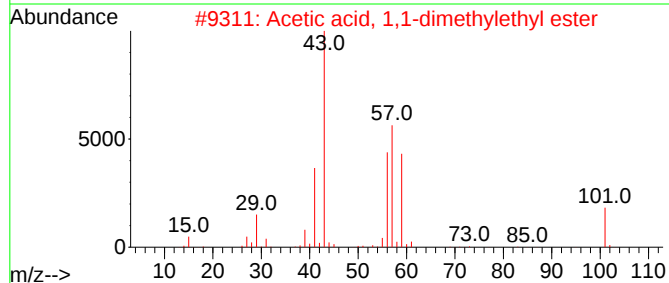
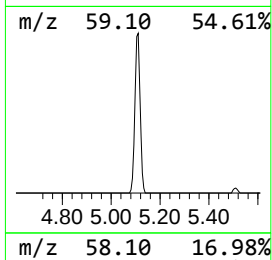
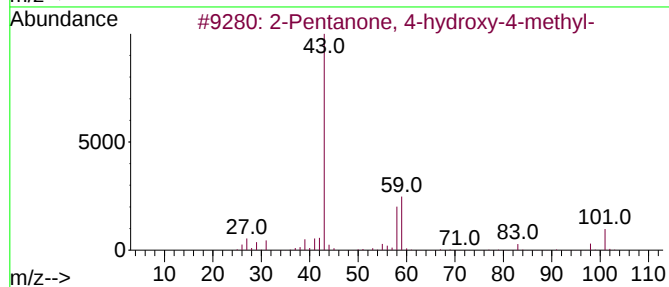
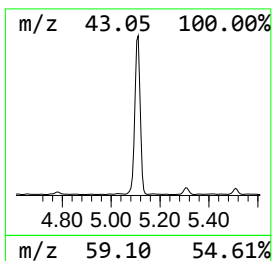
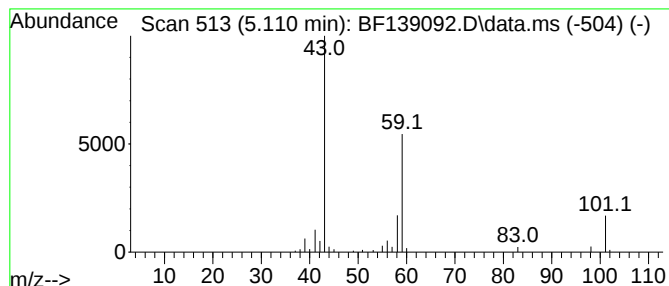
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	4.11 ng	112088	1,4-Dichlorobenzene-d4	6.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
5			Acetone	58	C3H6O	000067-64-1	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
Data File : BF139092.D
Acq On : 21 Aug 2024 10:22
Operator : RC/JU
Sample : P3663-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
916-J-SD-0.5-1-081624

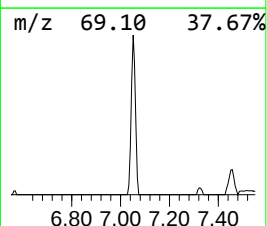
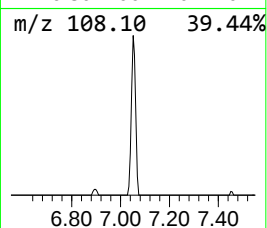
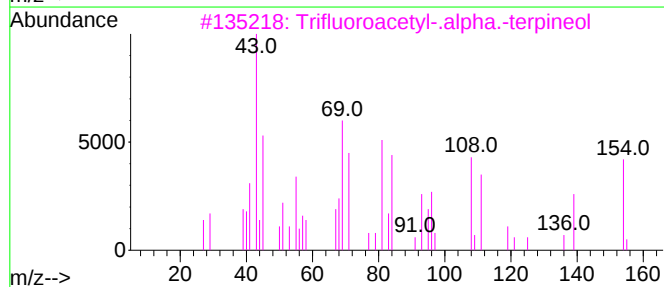
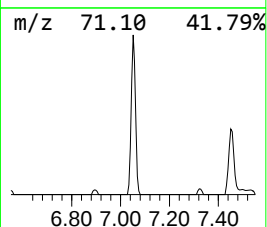
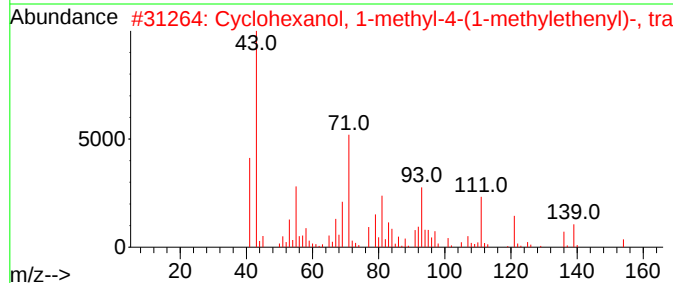
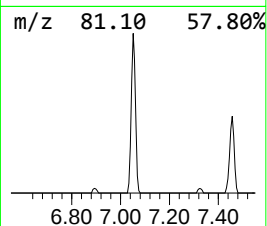
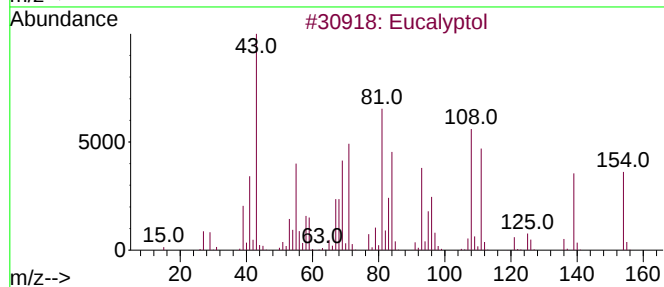
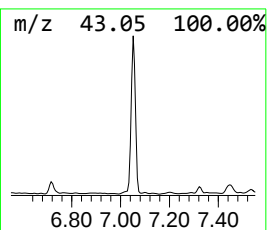
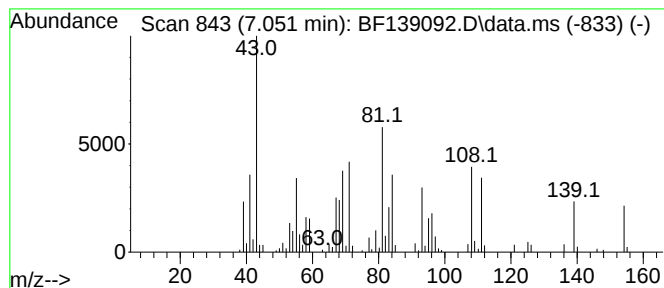
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Eucalyptol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.051	7.17 ng	195691	1,4-Dichlorobenzene-d4	6.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eucalyptol	154	C10H18O	000470-82-6	97
2			Cyclohexanol, 1-methyl-4-(1-meth...	154	C10H18O	007299-40-3	43
3			Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	38
4			4-Isopropyl-1-methylcyclohex-2-enol	154	C10H18O	000619-62-5	37
5			2-Isopropyl-5-methylhex-2-enal	154	C10H18O	035158-25-9	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
Data File : BF139092.D
Acq On : 21 Aug 2024 10:22
Operator : RC/JU
Sample : P3663-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

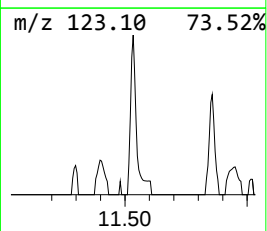
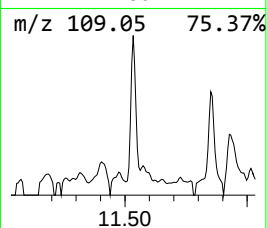
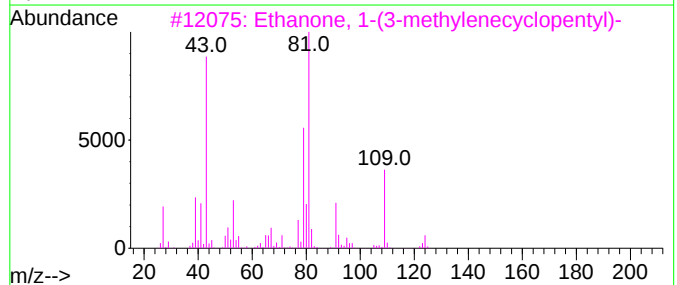
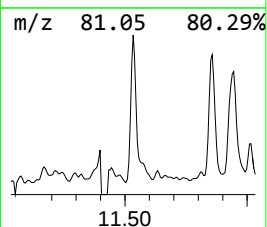
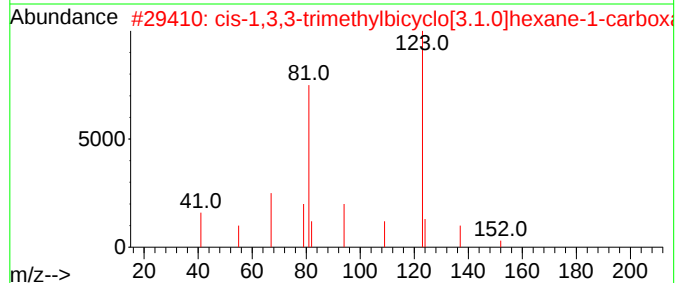
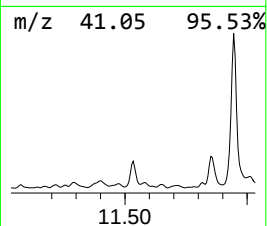
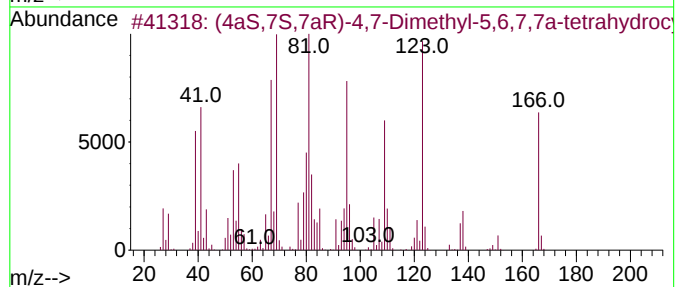
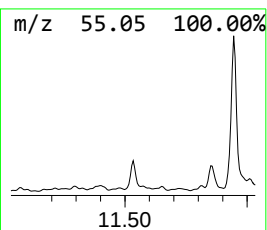
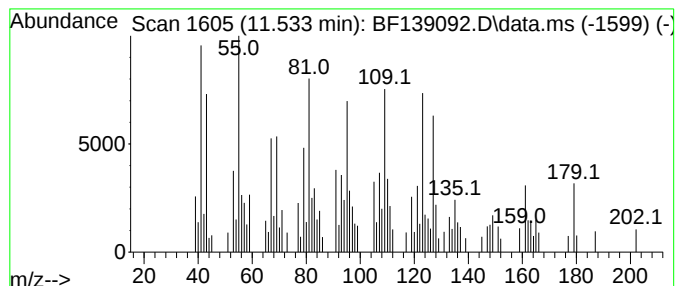
Instrument :
BNA_F
ClientSampleId :
916-J-SD-0.5-1-081624

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown11.533 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.533	2.02 ng	79960	Phenanthrene-d10	11.416	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(4aS,7S,7aR)-4,7-Dimethyl-5,6,7,...	166	C10H14O2	021651-62-7	49
2	cis-1,3,3-trimethylbicyclo[3.1.0...	152	C10H16O	1000365-94-2	30
3	Ethanone, 1-(3-methylenecyclopent...	124	C8H12O	054829-98-0	30
4	1,6,6-Trimethylbicyclo(3.3.0)oct...	166	C11H18O	1000427-23-1	20
5	1,1,6,6-Tetramethylspiro[4.4]nonane	180	C13H24	074054-92-5	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
Data File : BF139092.D
Acq On : 21 Aug 2024 10:22
Operator : RC/JU
Sample : P3663-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

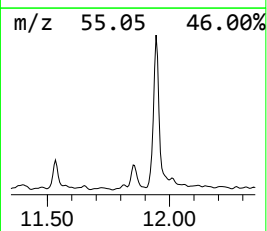
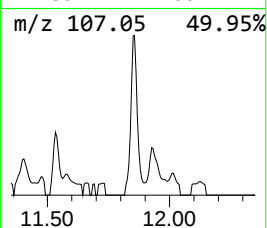
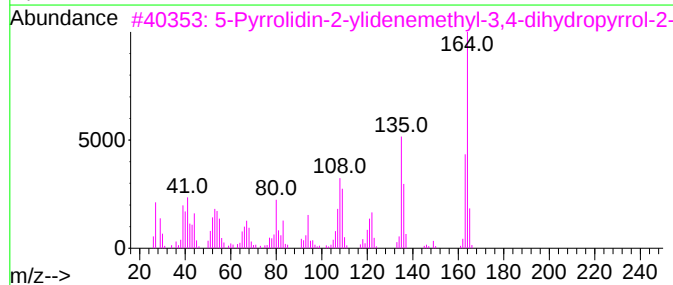
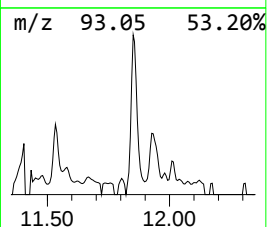
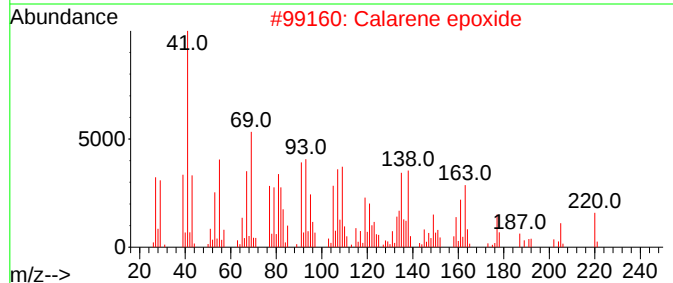
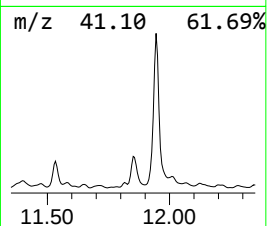
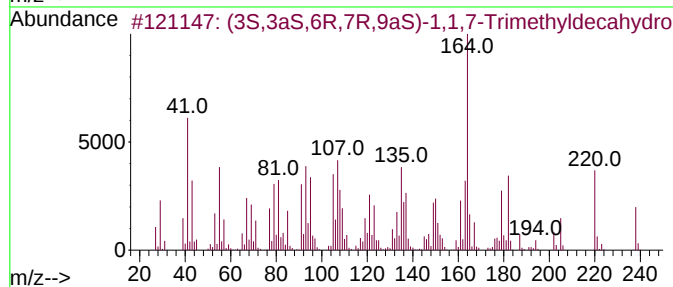
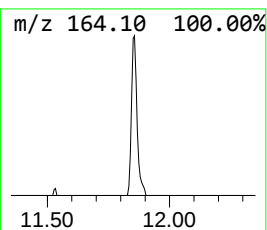
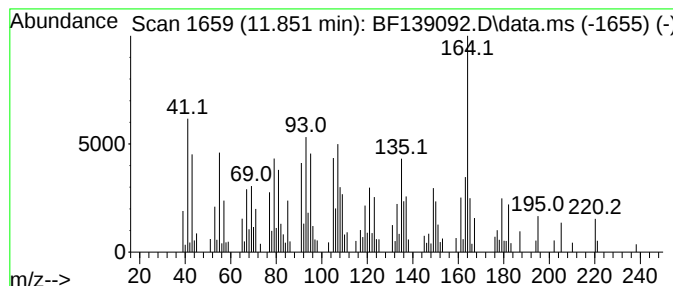
Instrument :
BNA_F
ClientSampleId :
916-J-SD-0.5-1-081624

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 (3S,3aS,6R,7R,9aS)-1,1,7-Tr... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.851	2.87 ng	113504	Phenanthrene-d10	11.416	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(3S,3aS,6R,7R,9aS)-1,1,7-Trimeth...	238	C15H26O2	002649-64-1	99
2	Calarene epoxide	220	C15H24O	1000151-46-0	46
3	5-Pyrrolidin-2-ylidenemethyl-3,4...	164	C9H12N2O	1010192-09-5	43
4	2-Benzothiazolamine, N-methyl-	164	C8H8N2S	016954-69-1	38
5	2-Phenylthiolane	164	C10H12S	002060-65-3	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
Data File : BF139092.D
Acq On : 21 Aug 2024 10:22
Operator : RC/JU
Sample : P3663-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
916-J-SD-0.5-1-081624

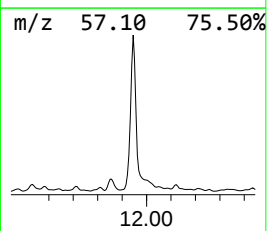
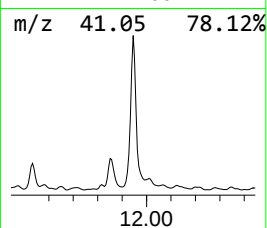
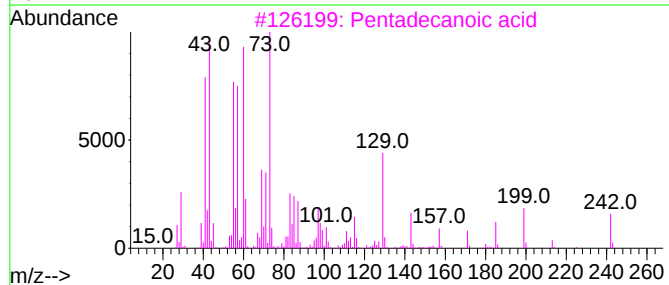
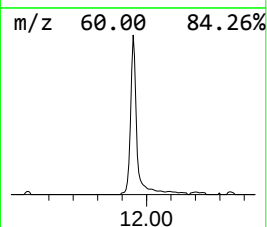
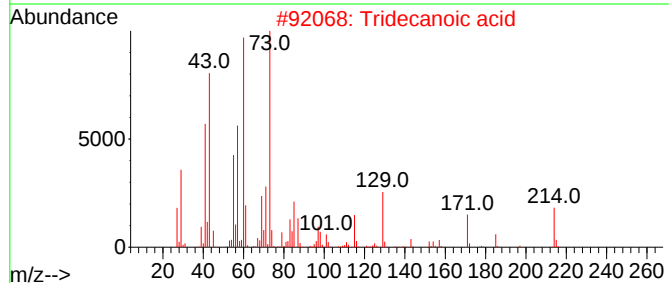
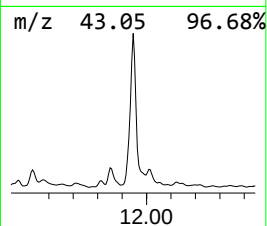
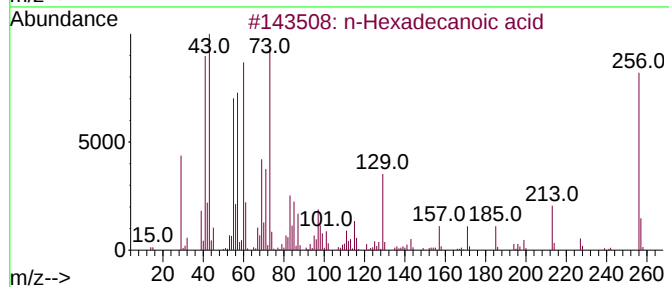
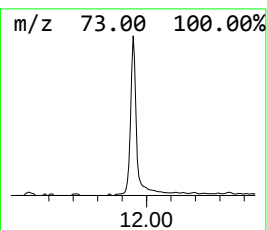
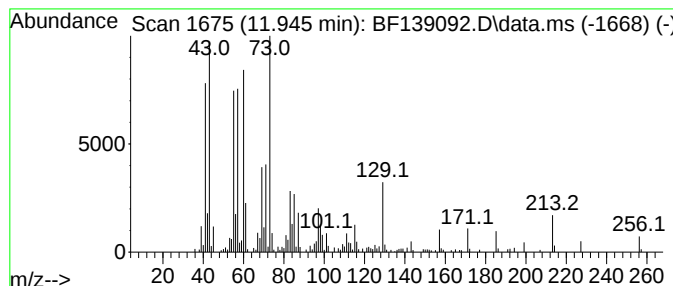
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.945	8.97 ng	354802	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	87
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
Data File : BF139092.D
Acq On : 21 Aug 2024 10:22
Operator : RC/JU
Sample : P3663-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
916-J-SD-0.5-1-081624

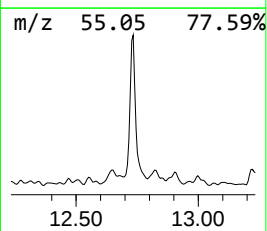
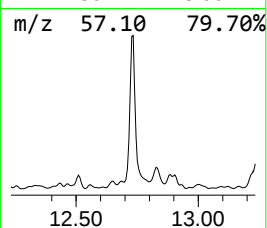
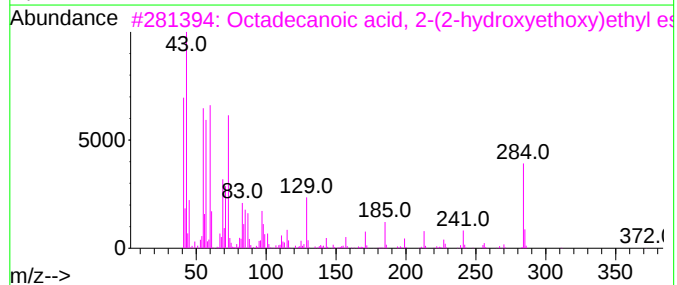
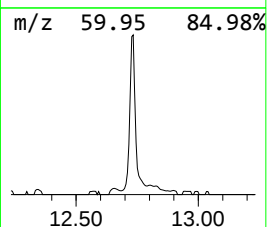
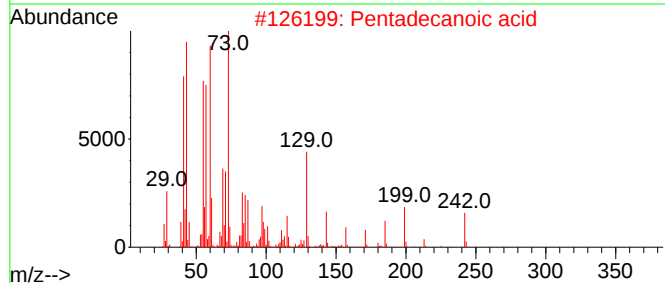
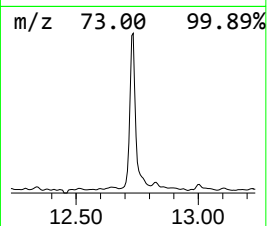
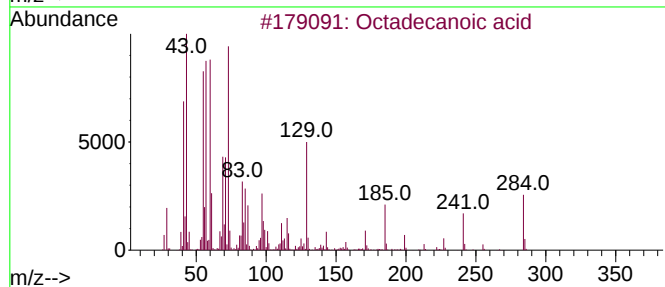
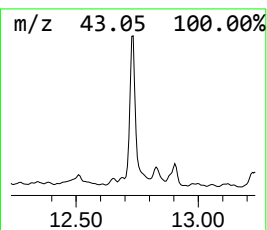
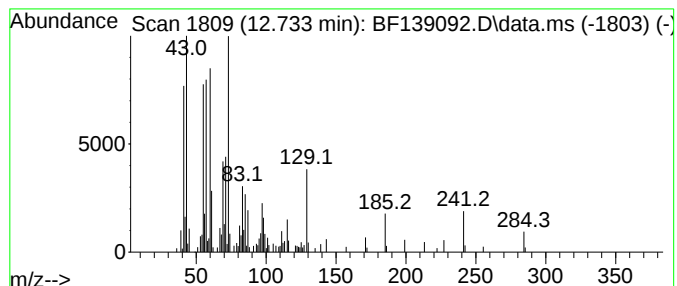
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.733	4.15 ng	164114	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	90
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
5			n-Decanoic acid	172	C10H20O2	000334-48-5	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
Data File : BF139092.D
Acq On : 21 Aug 2024 10:22
Operator : RC/JU
Sample : P3663-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
916-J-SD-0.5-1-081624

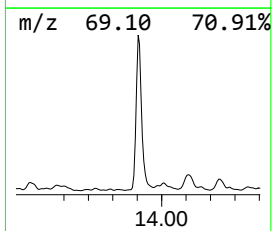
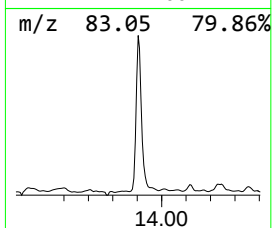
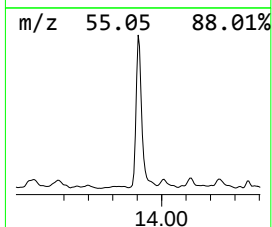
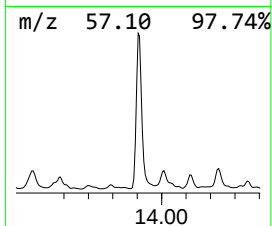
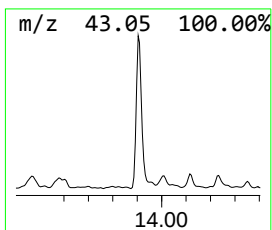
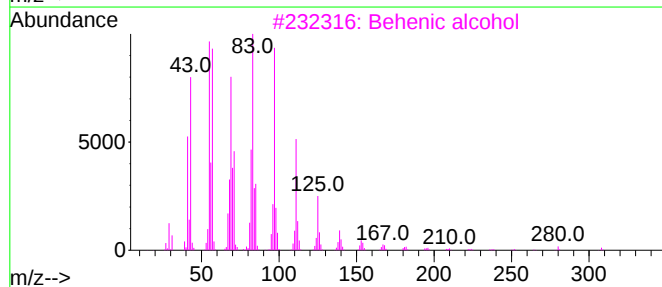
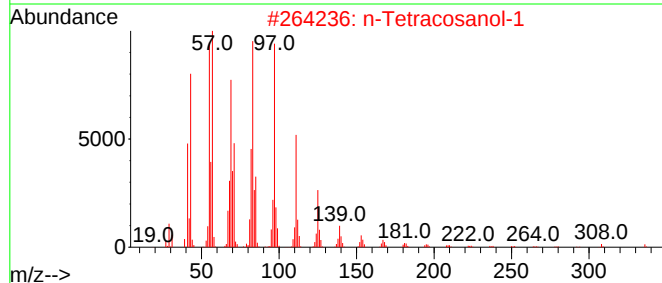
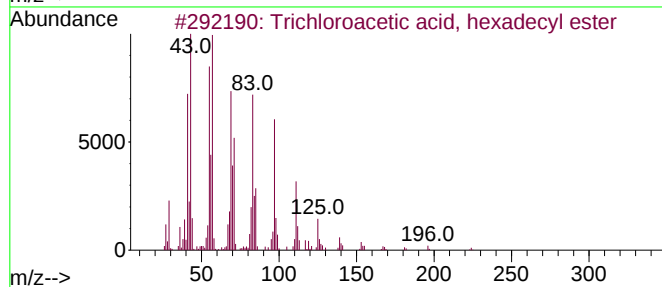
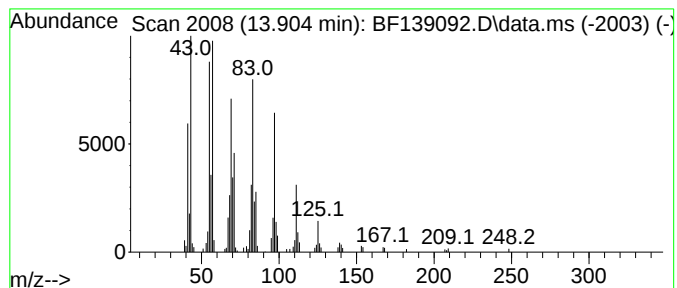
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Trichloroacetic acid, hexad... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	9.63 ng	192183	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	95
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3			Behenic alcohol	326	C22H46O	000661-19-8	94
4			1-Heneicosanol	312	C21H44O	015594-90-8	94
5			Octacosanol	410	C28H58O	000557-61-9	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
Data File : BF139092.D
Acq On : 21 Aug 2024 10:22
Operator : RC/JU
Sample : P3663-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

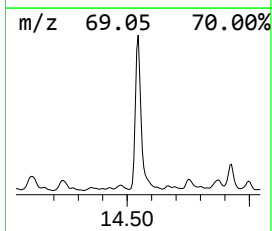
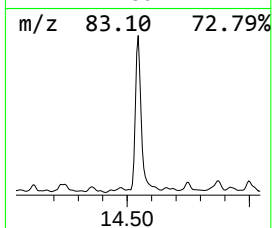
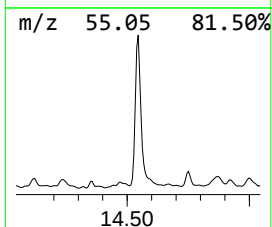
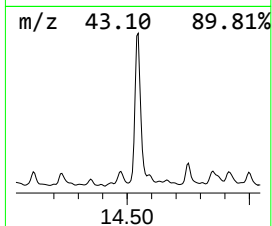
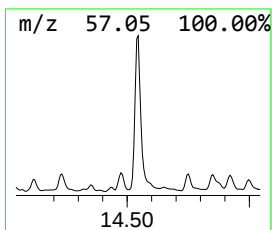
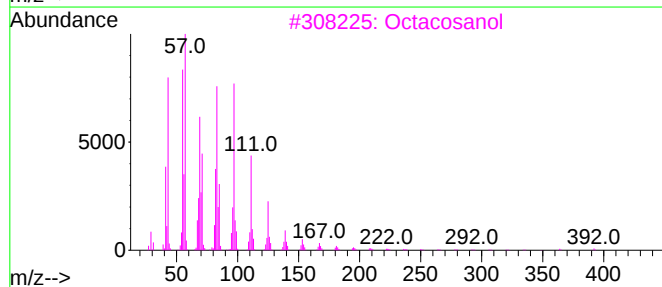
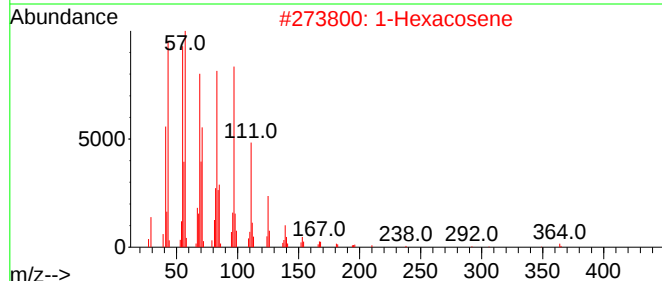
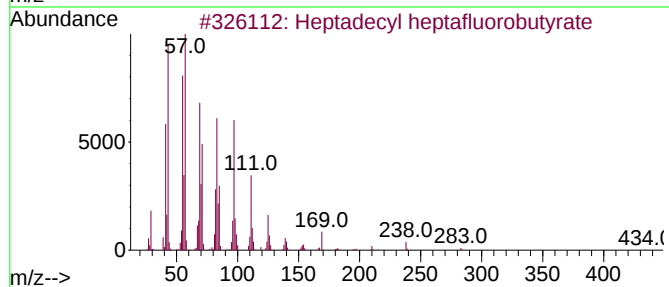
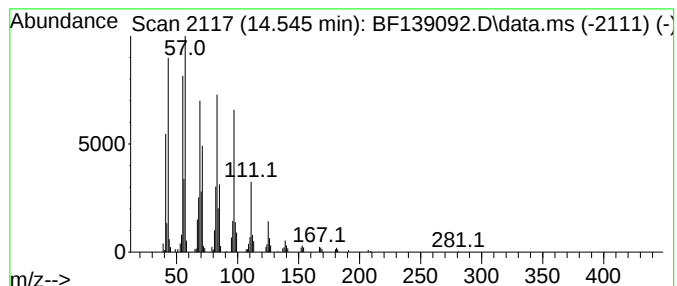
Instrument :
BNA_F
ClientSampleId :
916-J-SD-0.5-1-081624

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptadecyl heptafluorobutyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.545	10.59 ng	211317	Chrysene-d12		14.051	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate		452	C21H35F7O2	959085-66-6	94
2	1-Hexacosene		364	C26H52	018835-33-1	94
3	Octacosanol		410	C28H58O	000557-61-9	94
4	1-Heneicosanol		312	C21H44O	015594-90-8	93
5	n-Tetracosanol-1		354	C24H50O	000506-51-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
Data File : BF139092.D
Acq On : 21 Aug 2024 10:22
Operator : RC/JU
Sample : P3663-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
916-J-SD-0.5-1-081624

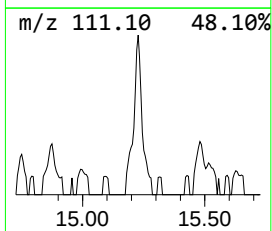
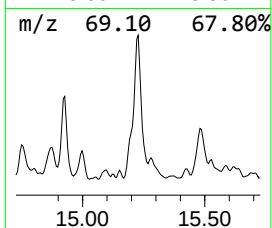
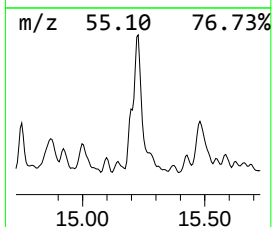
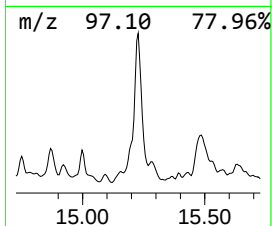
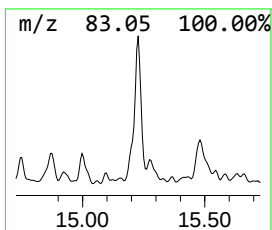
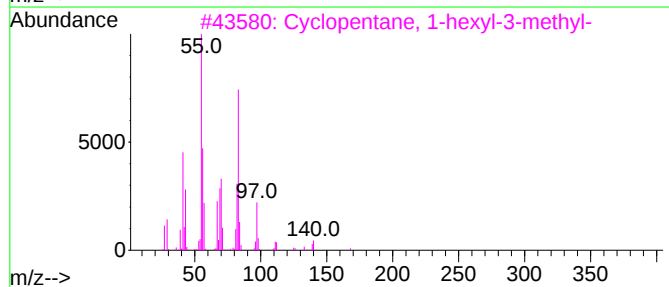
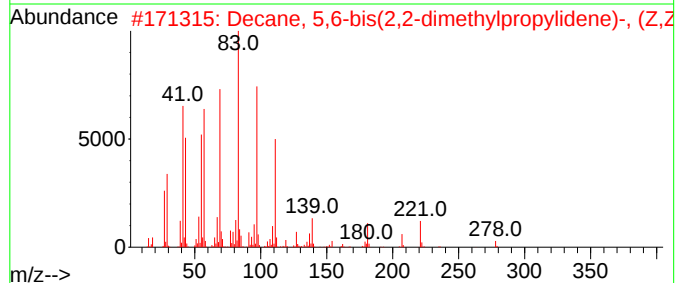
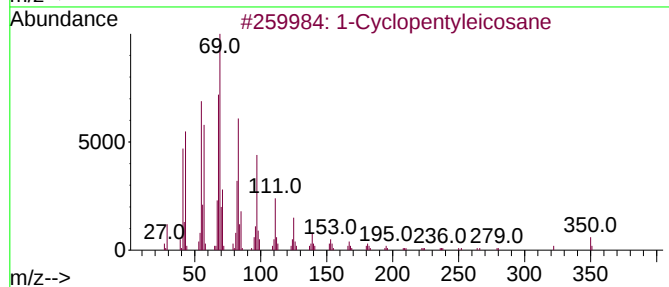
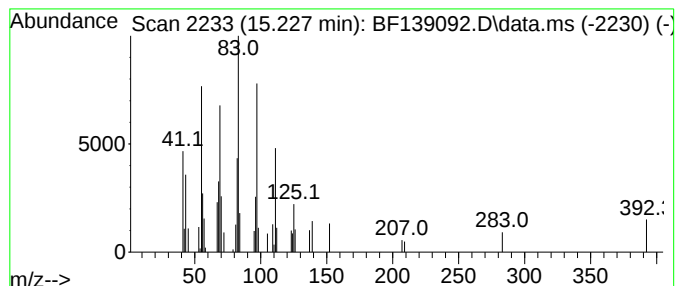
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1-Cyclopentyleicosane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.227	2.15 ng	52505	Perylene-d12	15.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Cyclopentyleicosane	350	C25H50	1000357-25-6	64
2			Decane, 5,6-bis(2,2-dimethylprop...	278	C20H38	073002-85-4	52
3			Cyclopentane, 1-hexyl-3-methyl-	168	C12H24	061142-68-5	43
4			1-Methylbicyclo[3.3.0]octane-3,7...	152	C9H12O2	021170-08-1	41
5			3a,7a-Epoxy-1H-inden-4(5H)-one, ...	152	C9H12O2	039746-31-1	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
Data File : BF139092.D
Acq On : 21 Aug 2024 10:22
Operator : RC/JU
Sample : P3663-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
916-J-SD-0.5-1-081624

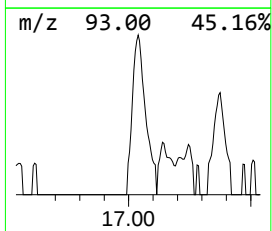
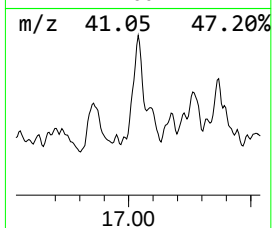
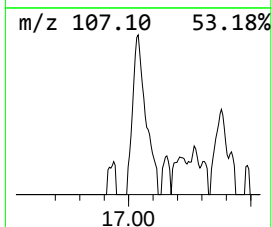
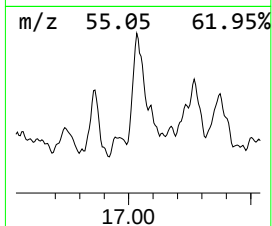
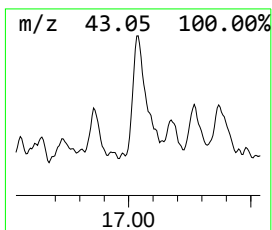
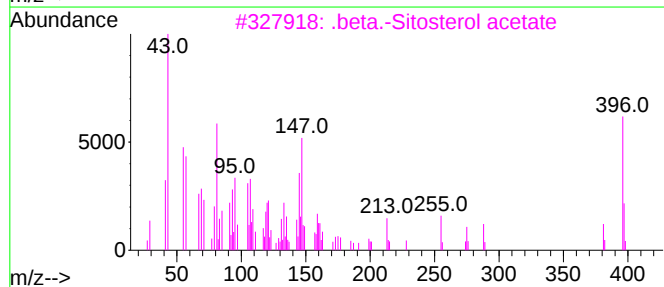
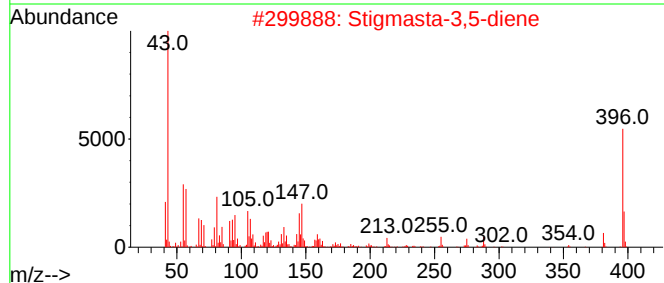
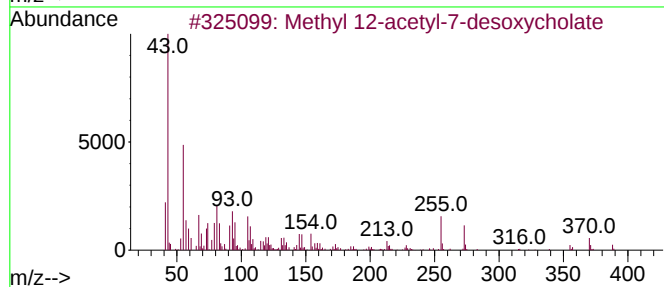
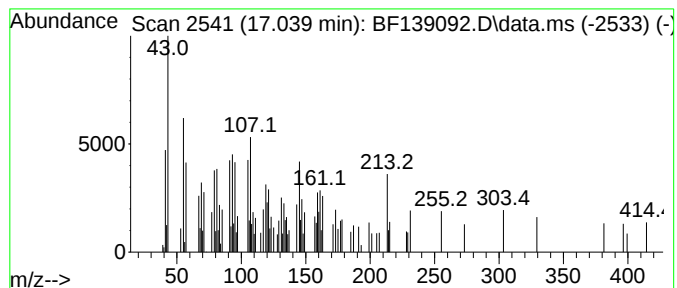
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown17.039 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.039	4.19 ng	102513	Perylene-d12	15.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl 12-acetyl-7-desoxycholate	448	C27H44O5	055547-48-3	35
2			Stigmasta-3,5-diene	396	C29H48	004970-37-0	35
3			.beta.-Sitosterol acetate	456	C31H52O2	000915-05-9	32
4			Pregn-5-en-3-ol, 21-bromo-20-met...	394	C22H35BrO	055103-80-5	27
5			5.beta.-Cholan-24-oic acid, 3-oxo-	374	C24H38O3	001553-56-6	16



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
Data File : BF139092.D
Acq On : 21 Aug 2024 10:22
Operator : RC/JU
Sample : P3663-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
916-J-SD-0.5-1-081624

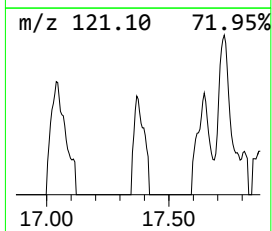
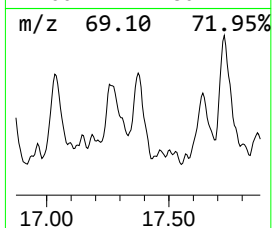
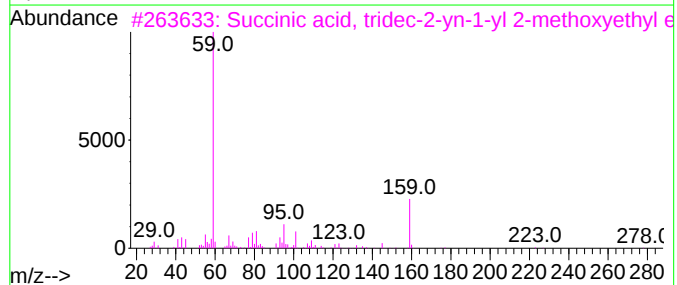
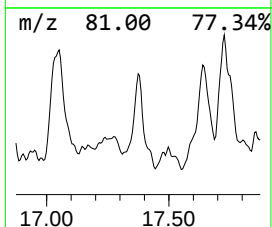
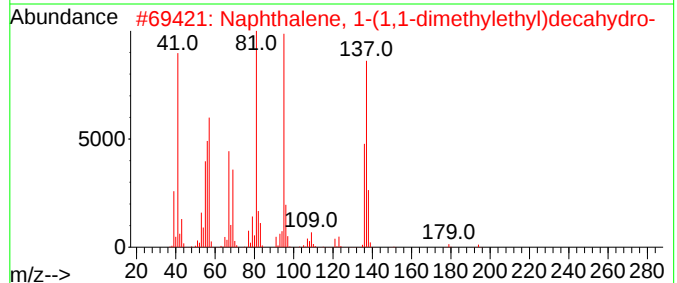
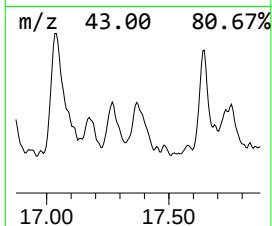
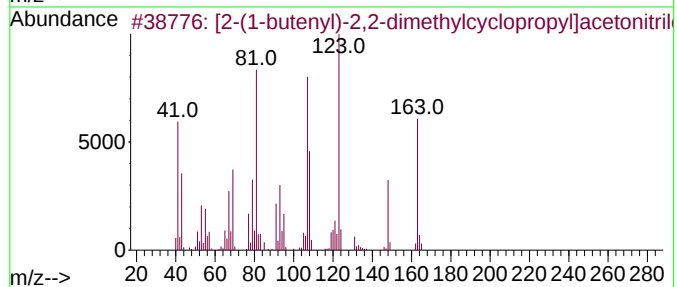
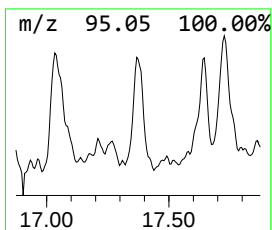
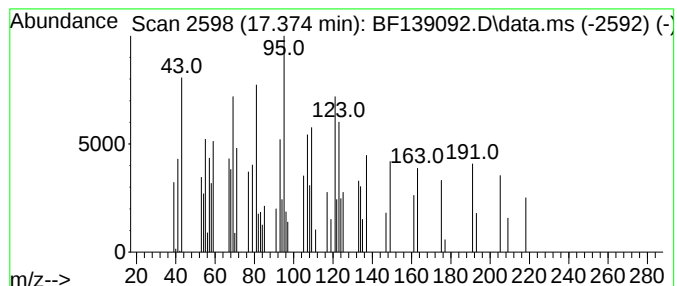
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown17.374 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.374	2.01 ng	49156	Perylene-d12	15.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			[2-(1-butenyl)-2,2-dimethylcyclo...	163	C11H17N	1000111-15-4	42
2			Naphthalene, 1-(1,1-dimethylethy...	194	C14H26	056292-64-9	35
3			Succinic acid, tridec-2-yn-1-yl ...	354	C20H34O5	1000390-75-1	27
4			2,2-Dimethylocta-3,4-dienal	152	C10H16O	000590-71-6	27
5			Cyclopentaneacetaldehyde, 2-form...	166	C10H14O2	005951-57-5	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
Data File : BF139092.D
Acq On : 21 Aug 2024 10:22
Operator : RC/JU
Sample : P3663-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
916-J-SD-0.5-1-081624

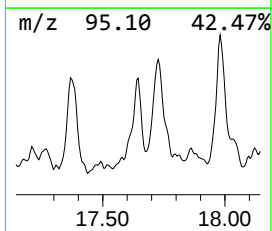
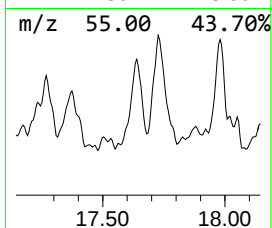
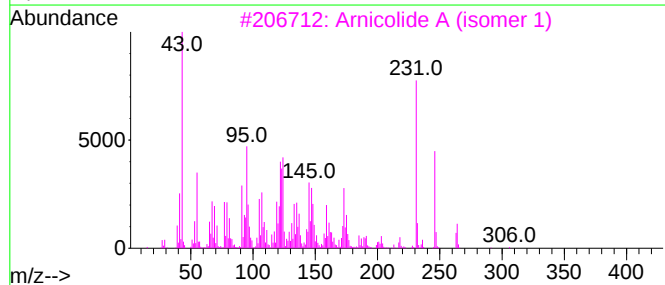
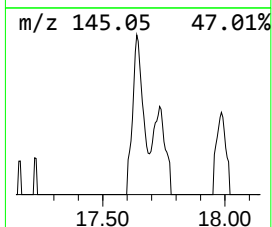
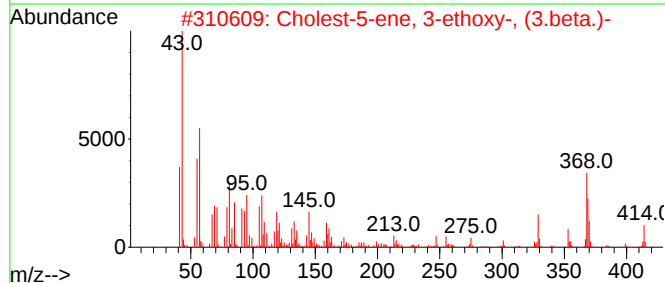
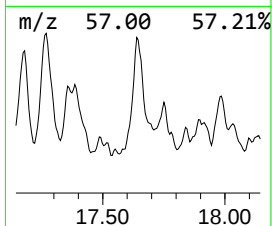
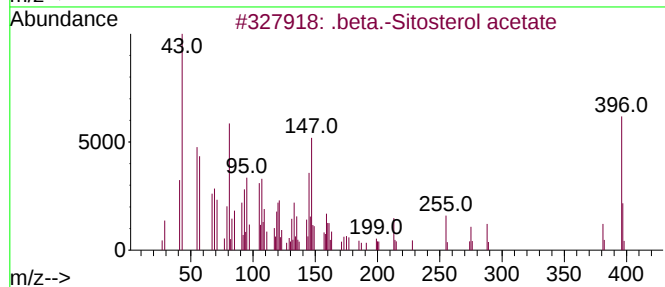
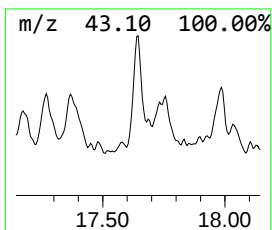
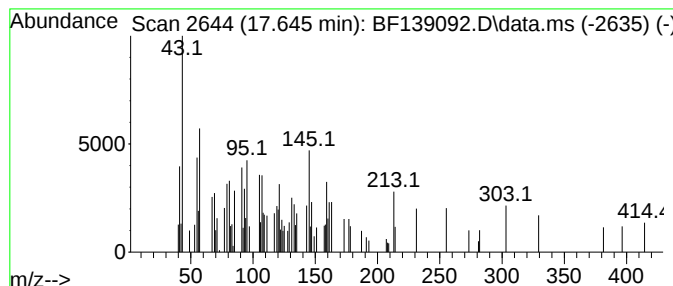
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown17.645 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.645	2.50 ng	61174	Perylene-d12	15.533

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		.beta.-Sitosterol acetate	456	C31H52O2	000915-05-9	38
2		Cholest-5-ene, 3-ethoxy-, (3.beta...	414	C29H50O	000986-19-6	30
3		Arnicolide A (isomer 1)	306	C17H22O5	1000495-69-7	14
4		Stigmastan-3-en-6-ol	414	C29H50O	1000214-19-7	10
5		Methyl 12-acetyl-7-desoxycholate	448	C27H44O5	055547-48-3	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
Data File : BF139092.D
Acq On : 21 Aug 2024 10:22
Operator : RC/JU
Sample : P3663-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
916-J-SD-0.5-1-081624

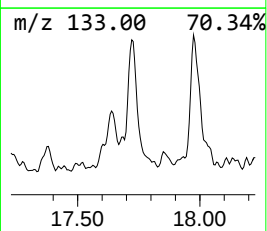
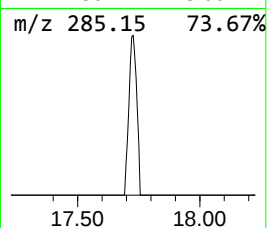
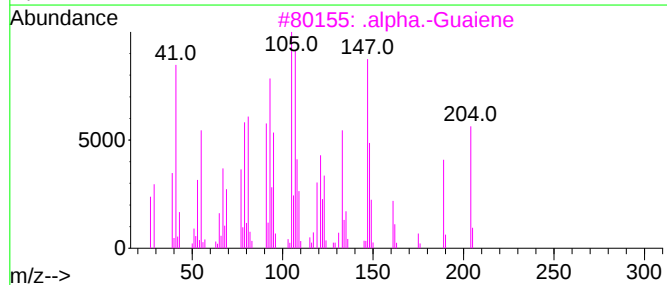
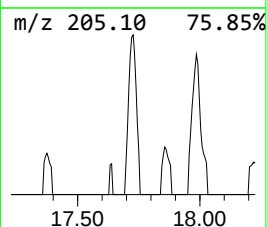
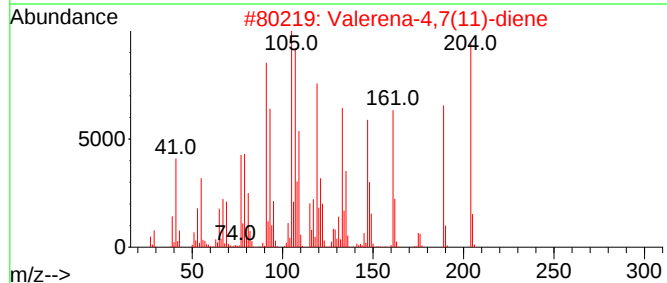
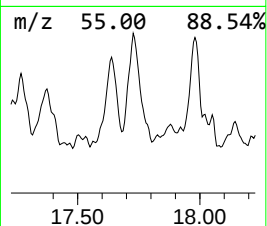
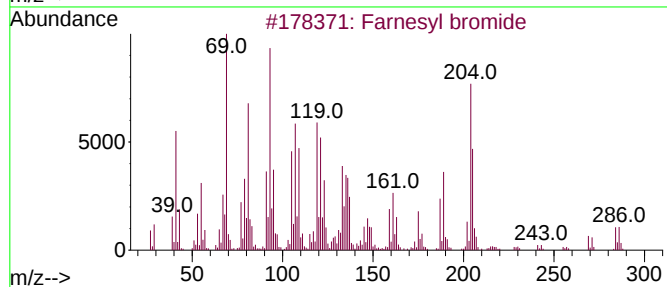
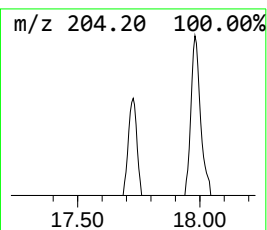
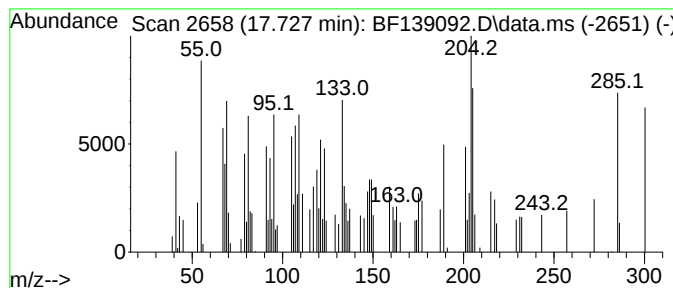
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 unknown17.727 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.727	3.88 ng	94827	Perylene-d12	15.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Farnesyl bromide	284	C15H25Br	006874-67-5	46
2			Valerena-4,7(11)-diene	204	C15H24	351222-66-7	38
3			.alpha.-Guaiene	204	C15H24	003691-12-1	38
4			1R,4S,7S,11R-2,2,4,8-Tetramethyl...	204	C15H24	1208118-28-8	38
5			Azulene, 1,2,3,3a,4,5,6,7-octahy...	204	C15H24	022567-17-5	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
Data File : BF139092.D
Acq On : 21 Aug 2024 10:22
Operator : RC/JU
Sample : P3663-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
916-J-SD-0.5-1-081624

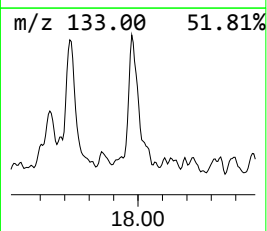
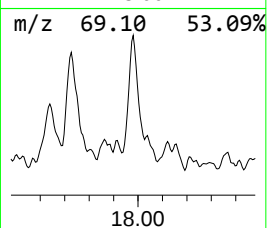
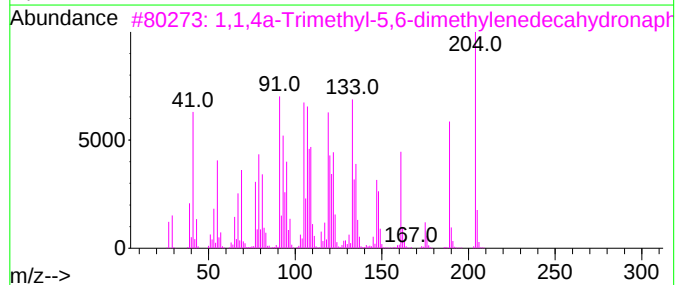
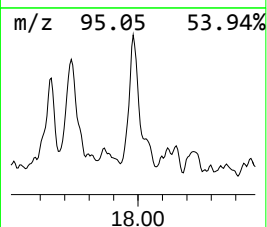
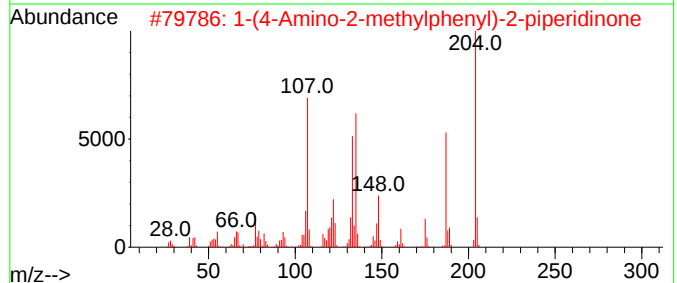
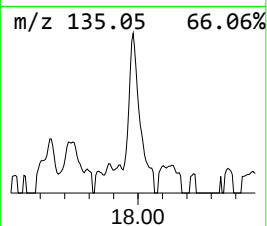
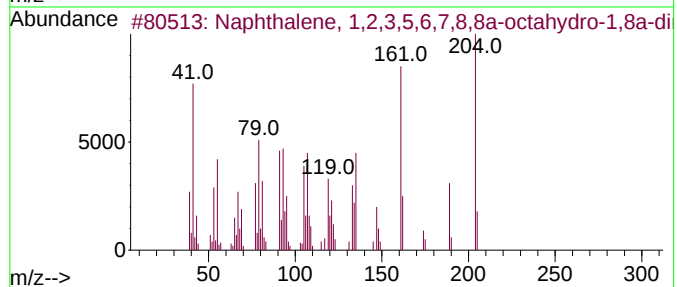
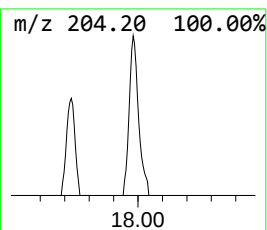
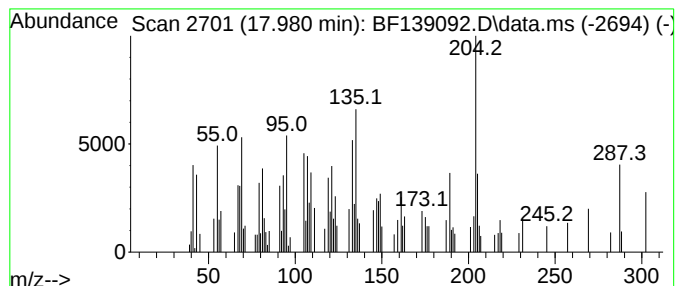
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Naphthalene, 1,2,3,5,6,7,8,... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.980	4.90 ng	119698	Perylene-d12	15.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	70
2			1-(4-Amino-2-methylphenyl)-2-pip...	204	C12H16N2O	443999-53-9	49
3			1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	49
4			1H-Cycloprop[e]azulene, 1a,2,3,4...	204	C15H24	000489-40-7	38
5			Naphthalene, decahydro-4a-methyl...	204	C15H24	017066-67-0	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082124\
Data File : BF139092.D
Acq On : 21 Aug 2024 10:22
Operator : RC/JU
Sample : P3663-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
916-J-SD-0.5-1-081624

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.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
Butane, 2-metho...	2.193	67.8	ng	1851820	1	6.898	545955	20.0
R-(-)-1,2-propa...	3.393	2.8	ng	76975	1	6.898	545955	20.0
2-Pentanone, 4-...	5.110	4.1	ng	112088	1	6.898	545955	20.0
Eucalyptol	7.051	7.2	ng	195691	1	6.898	545955	20.0
unknown11.533	11.533	2.0	ng	79960	4	11.416	791458	20.0
(3S,3aS,6R,7R,9...	11.851	2.9	ng	113504	4	11.416	791458	20.0
n-Hexadecanoic ...	11.945	9.0	ng	354802	4	11.416	791458	20.0
Octadecanoic acid	12.733	4.2	ng	164114	4	11.416	791458	20.0
Trichloroacetic...	13.904	9.6	ng	192183	5	14.051	399101	20.0
Heptadecyl hept...	14.545	10.6	ng	211317	5	14.051	399101	20.0
1-Cyclopentylei...	15.227	2.1	ng	52505	6	15.533	488935	20.0
unknown17.039	17.039	4.2	ng	102513	6	15.533	488935	20.0
unknown17.374	17.374	2.0	ng	49156	6	15.533	488935	20.0
unknown17.645	17.645	2.5	ng	61174	6	15.533	488935	20.0
unknown17.727	17.727	3.9	ng	94827	6	15.533	488935	20.0
Naphthalene, 1,...	17.980	4.9	ng	119698	6	15.533	488935	20.0