

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081524\
 Data File : BF139027.D
 Acq On : 15 Aug 2024 17:37
 Operator : RC/JU
 Sample : P3580-03
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 925-K1-SD-0-0.5-081224

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-BF073024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139027.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.481	56	66	76	rVB	72229	127066	14.79%	1.989%
2	4.557	415	419	424	rBB	13617	19516	2.27%	0.305%
3	5.057	499	504	517	rBV	33509	54287	6.32%	0.850%
4	5.469	569	574	599	rBV	583232	816718	95.09%	12.782%
5	6.481	741	746	763	rBV	630978	858873	100.00%	13.442%
6	6.834	802	806	815	rBB	195236	235973	27.47%	3.693%
7	6.981	827	831	835	rVB	14376	16098	1.87%	0.252%
8	7.398	897	902	921	rBV	413499	548969	63.92%	8.592%
9	7.663	943	947	956	rBV	9091	15533	1.81%	0.243%
10	8.116	1019	1024	1031	rBV	243304	301959	35.16%	4.726%
11	8.433	1074	1078	1090	rBV	29461	48320	5.63%	0.756%
12	9.186	1201	1206	1211	rBV	705978	858544	99.96%	13.437%
13	9.575	1267	1272	1277	rBV2	6059	10390	1.21%	0.163%
14	9.869	1317	1322	1329	rVB	262387	340268	39.62%	5.325%
15	9.957	1332	1337	1342	rVB	18438	27547	3.21%	0.431%
16	10.504	1425	1430	1434	rBV	12722	17565	2.05%	0.275%
17	10.657	1452	1456	1465	rBV	402767	516733	60.16%	8.087%
18	10.769	1470	1475	1483	rVB	25676	37541	4.37%	0.588%
19	11.098	1526	1531	1536	rBV5	5712	14344	1.67%	0.224%
20	11.233	1550	1554	1561	rVB	18289	27328	3.18%	0.428%
21	11.357	1570	1575	1588	rVB	261682	350508	40.81%	5.486%
22	11.792	1646	1649	1658	rVB9	3814	8935	1.04%	0.140%
23	11.874	1658	1663	1674	rVB10	7023	17788	2.07%	0.278%
24	12.933	1838	1843	1848	rBV	493242	597714	69.59%	9.355%
25	13.210	1886	1890	1896	rVB	12252	14236	1.66%	0.223%
26	13.827	1989	1995	2012	rBV5	14019	46886	5.46%	0.734%
27	13.998	2019	2024	2034	rVB	144508	187621	21.85%	2.936%
28	14.445	2095	2100	2103	rBV2	11346	17141	2.00%	0.268%
29	15.074	2202	2207	2212	rVB	21516	29757	3.46%	0.466%
30	15.462	2267	2273	2283	rBV	117941	188955	22.00%	2.957%
31	15.874	2337	2343	2350	rBV	14047	25869	3.01%	0.405%
32	16.656	2471	2476	2482	rBV6	5768	10508	1.22%	0.164%

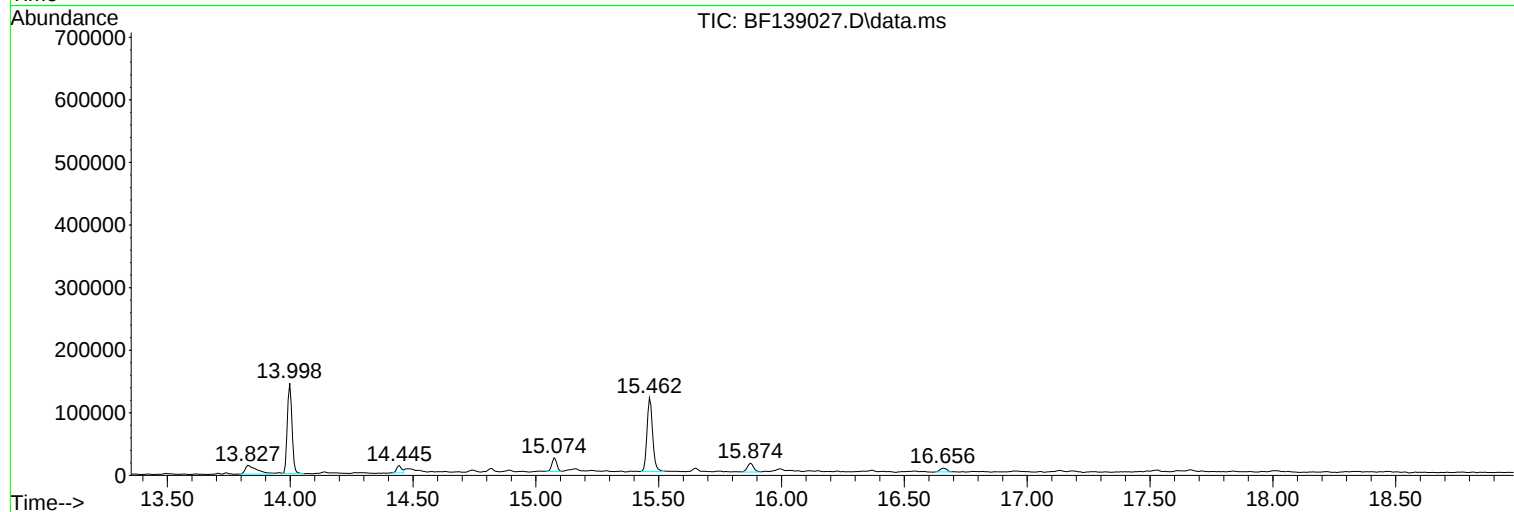
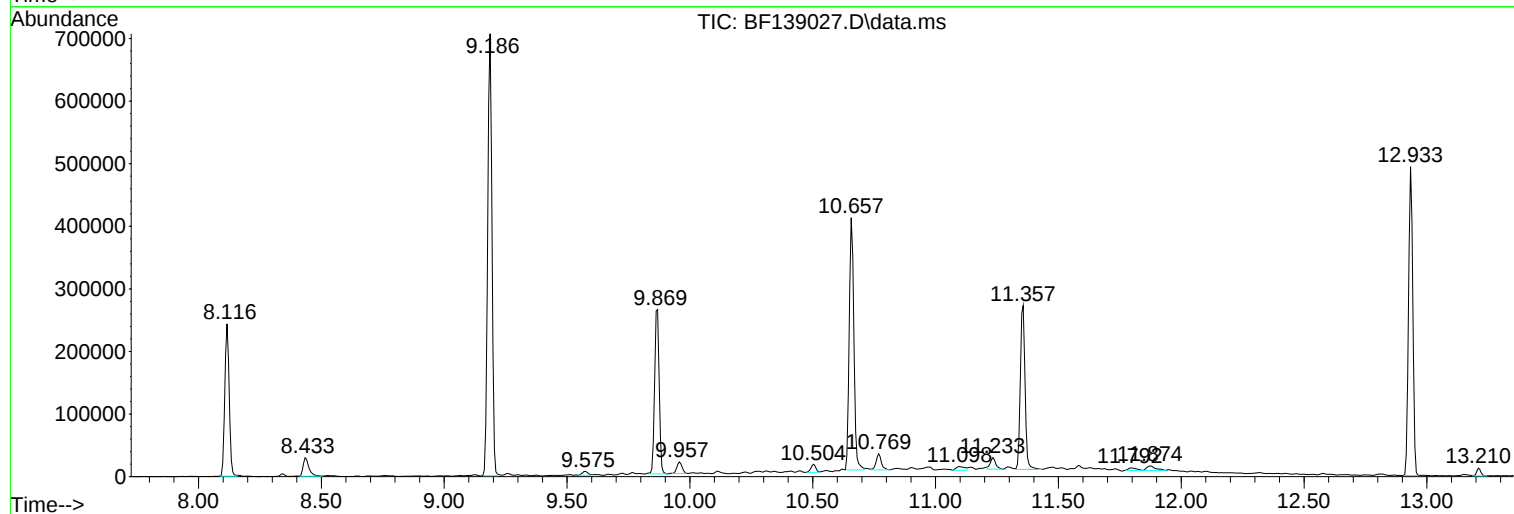
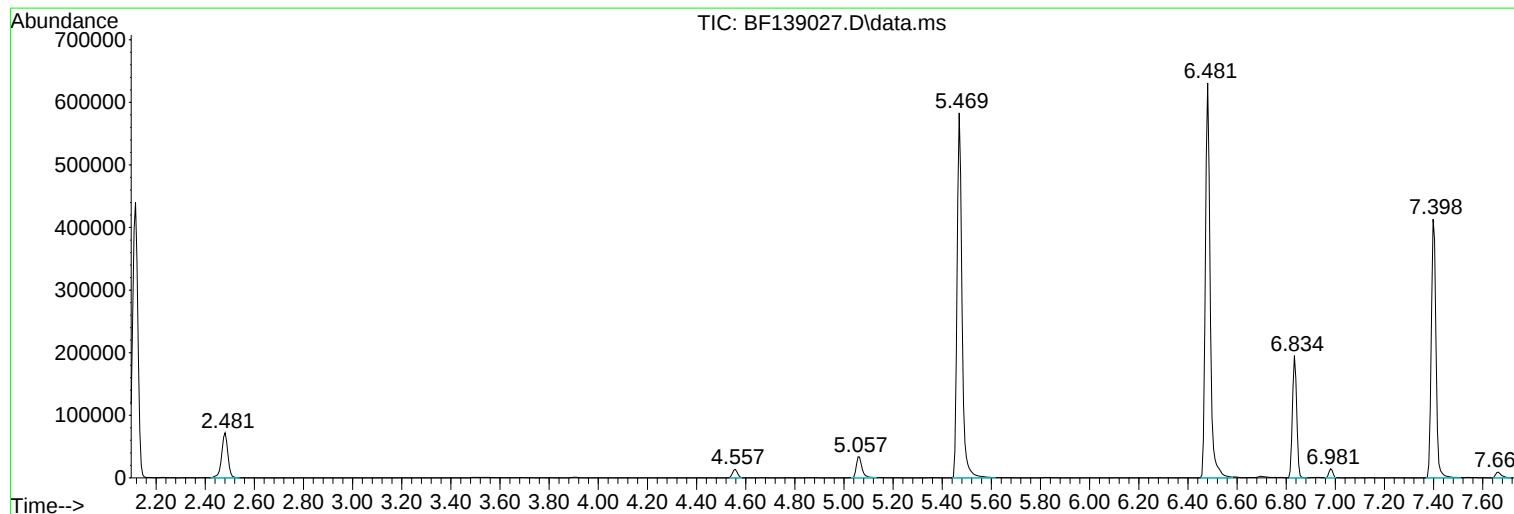
Sum of corrected areas: 6389490

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081524\
Data File : BF139027.D
Acq On : 15 Aug 2024 17:37
Operator : RC/JU
Sample : P3580-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
925-K1-SD-0-0.5-081224

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.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\BF081524\
Data File : BF139027.D
Acq On : 15 Aug 2024 17:37
Operator : RC/JU
Sample : P3580-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
925-K1-SD-0-0.5-081224

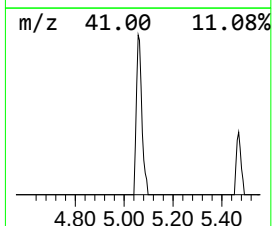
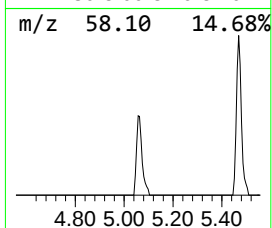
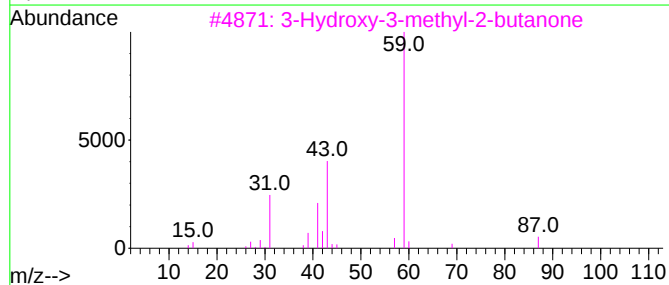
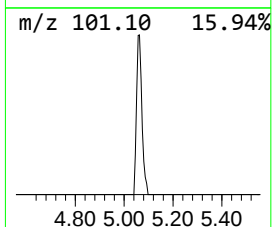
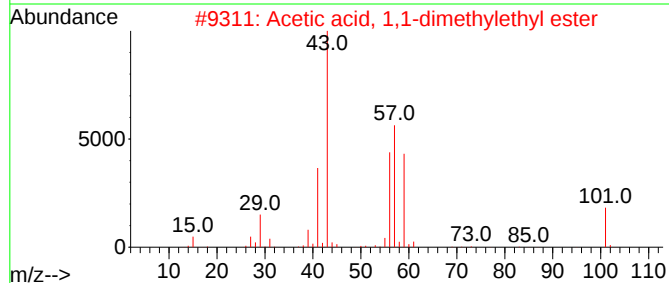
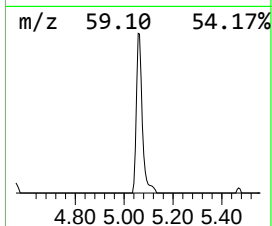
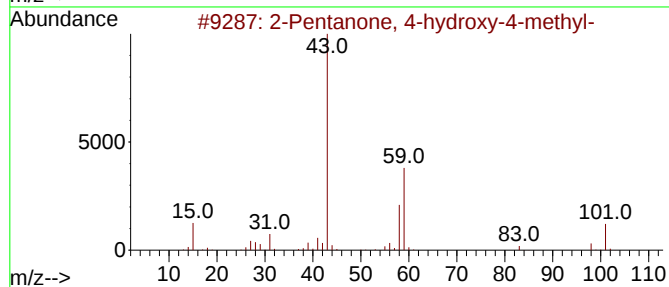
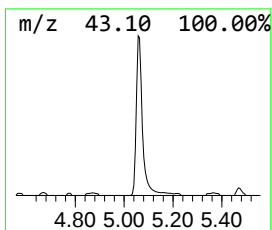
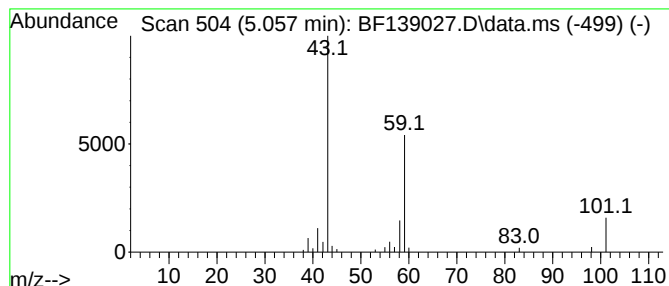
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.057	4.60 ng	54287	1,4-Dichlorobenzene-d4	6.834

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	37
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081524\
Data File : BF139027.D
Acq On : 15 Aug 2024 17:37
Operator : RC/JU
Sample : P3580-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
925-K1-SD-0-0.5-081224

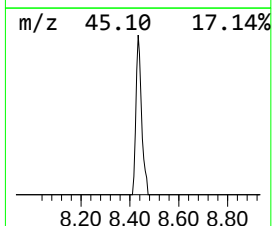
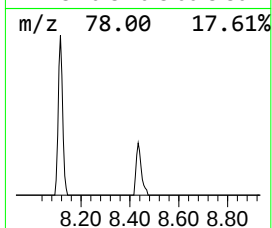
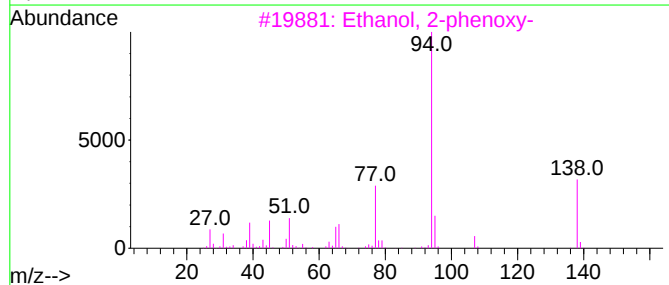
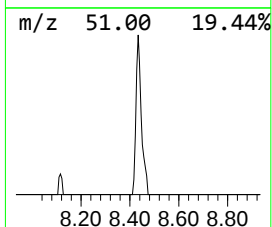
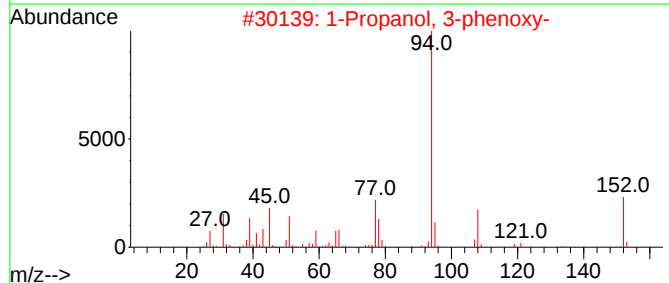
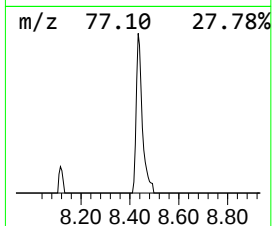
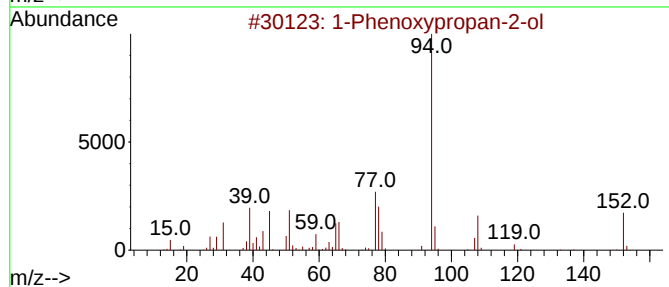
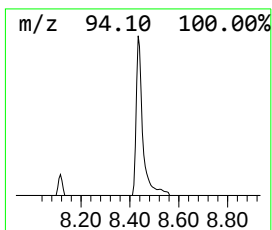
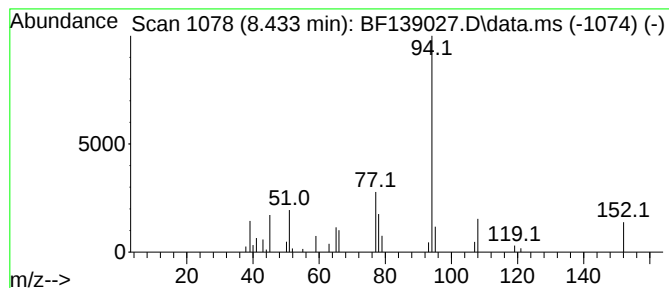
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.433	3.20 ng	48320	Naphthalene-d8	8.116

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	90
3		Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4		Pyrimidine, 5-methyl-	94	C5H6N2	002036-41-1	50
5		2-Hexen-4-yne, 2-methyl-	94	C7H10	058275-93-7	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081524\
Data File : BF139027.D
Acq On : 15 Aug 2024 17:37
Operator : RC/JU
Sample : P3580-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
925-K1-SD-0-0.5-081224

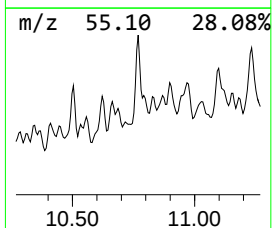
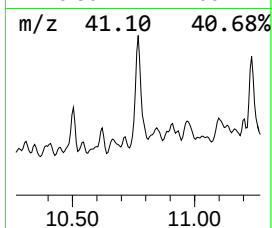
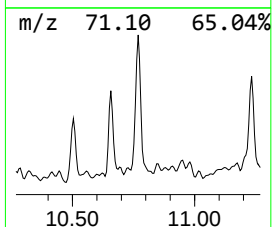
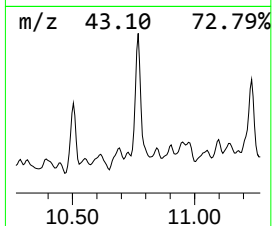
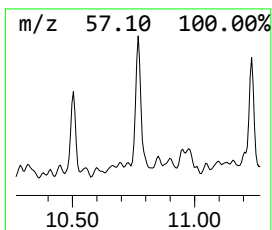
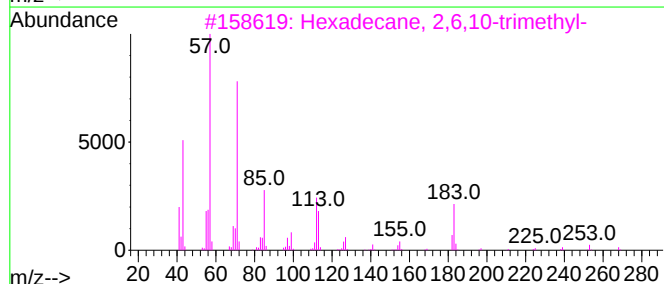
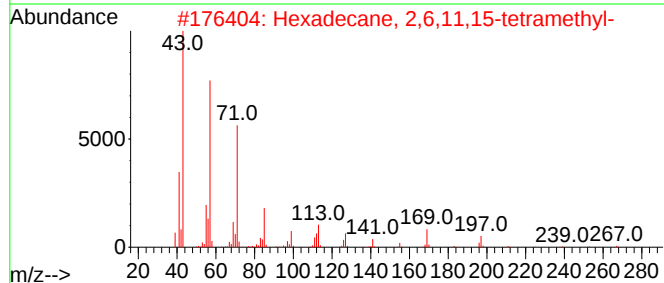
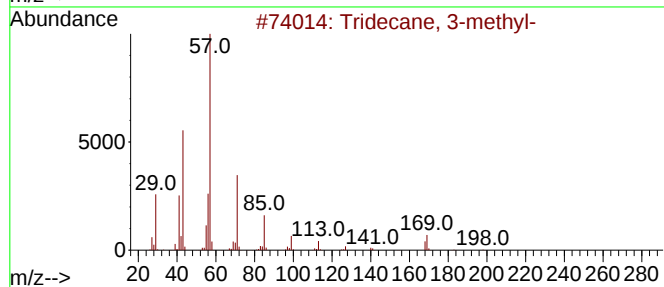
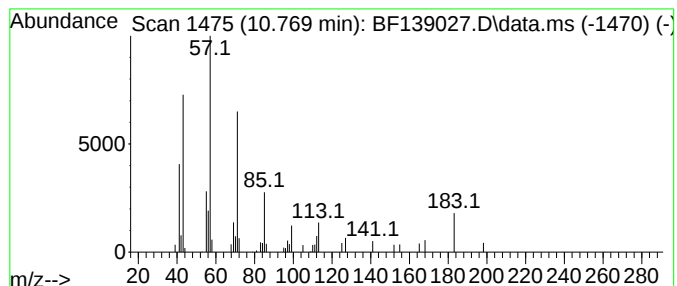
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Tridecane, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.769	2.14 ng	37541	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane, 3-methyl-	198	C14H30	006418-41-3	80
2			Hexadecane, 2,6,11,15-tetramethyl-	282	C20H42	000504-44-9	72
3			Hexadecane, 2,6,10-trimethyl-	268	C19H40	055000-52-7	64
4			Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	59
5			Undecane, 3,8-dimethyl-	184	C13H28	017301-30-3	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081524\
Data File : BF139027.D
Acq On : 15 Aug 2024 17:37
Operator : RC/JU
Sample : P3580-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
925-K1-SD-0-0.5-081224

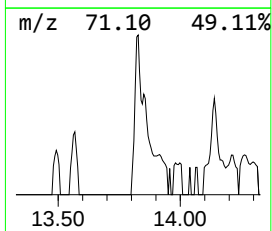
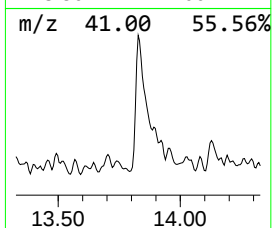
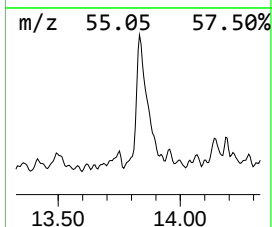
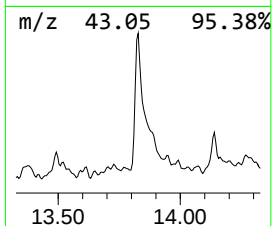
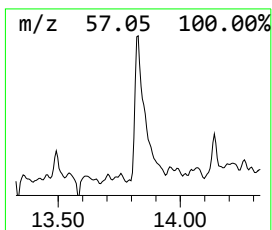
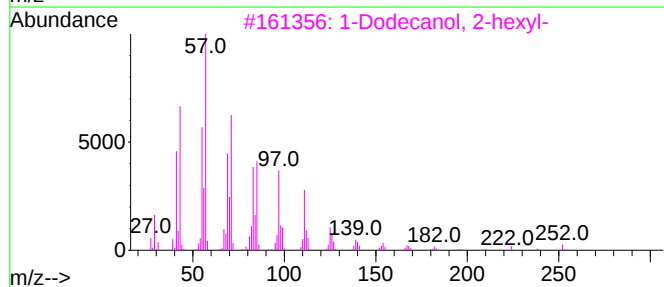
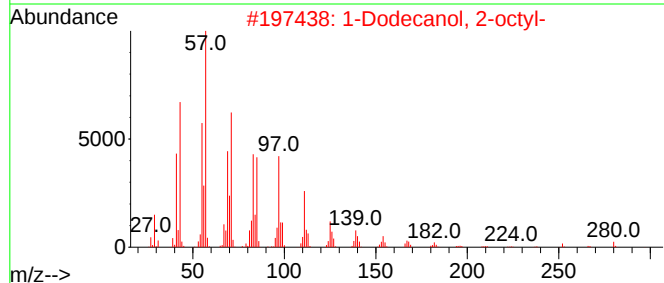
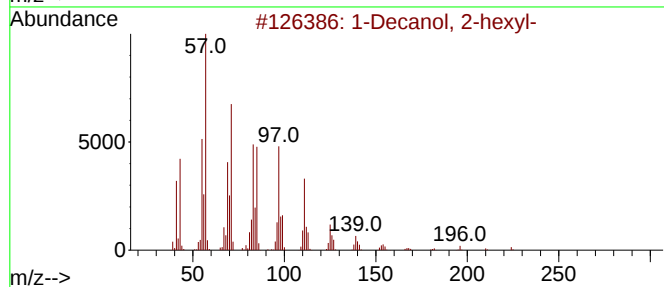
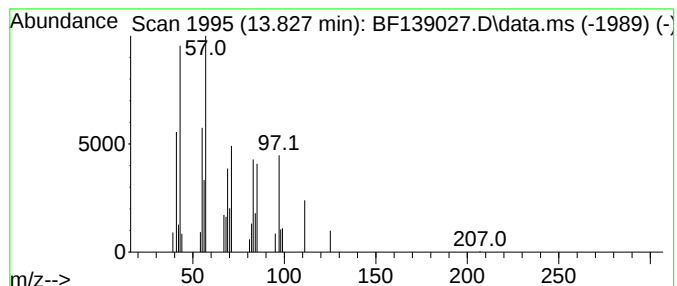
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1-Decanol, 2-hexyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.827	5.00 ng	46886	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	90
2			1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	90
3			1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	86
4			1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	86
5			Oxalic acid, cyclobutyl pentadec...	354	C21H38O4	1010309-70-5	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081524\
Data File : BF139027.D
Acq On : 15 Aug 2024 17:37
Operator : RC/JU
Sample : P3580-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
925-K1-SD-0-0.5-081224

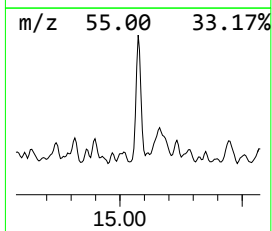
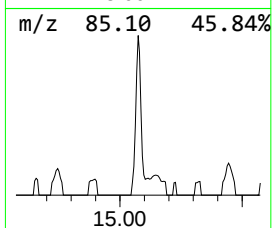
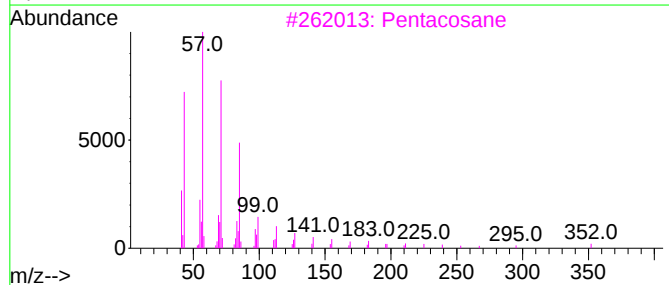
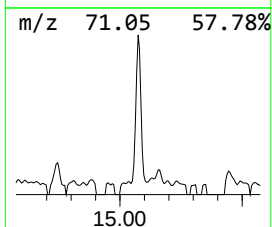
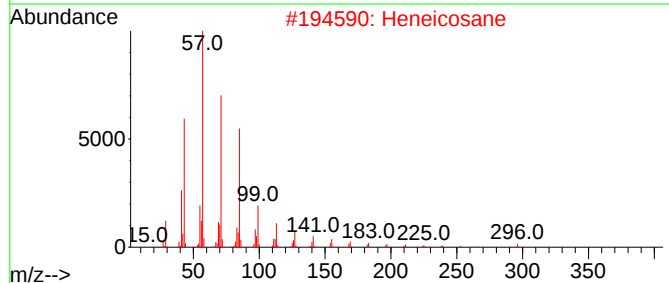
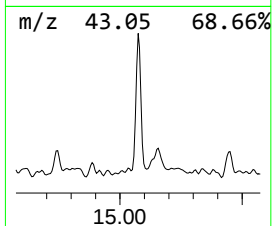
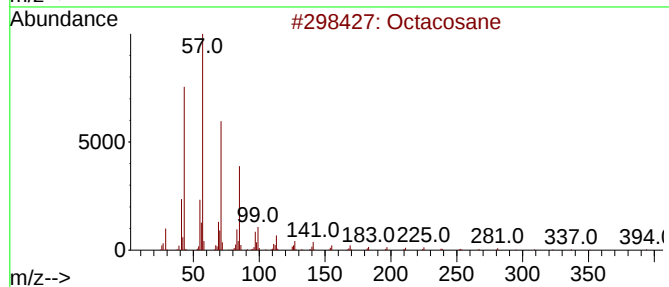
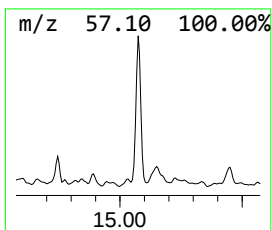
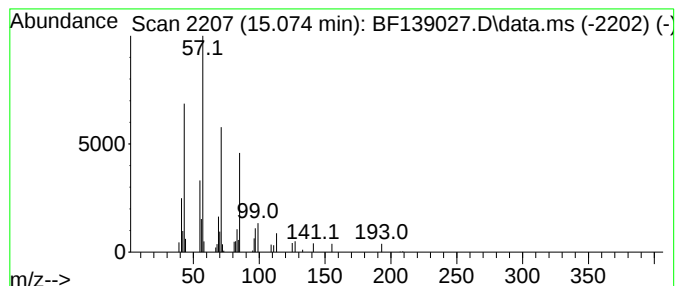
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.074	3.15 ng	29757	Perylene-d12	15.462

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosane	394	C28H58	000630-02-4	87
2		Heneicosane	296	C21H44	000629-94-7	87
3		Pentacosane	352	C25H52	000629-99-2	87
4		Tetratetracontane	619	C44H90	007098-22-8	86
5		Hexatriacontane	507	C36H74	000630-06-8	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081524\
Data File : BF139027.D
Acq On : 15 Aug 2024 17:37
Operator : RC/JU
Sample : P3580-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
925-K1-SD-0-0.5-081224

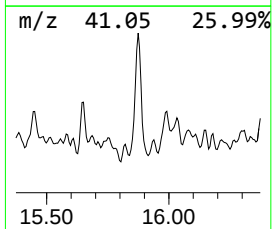
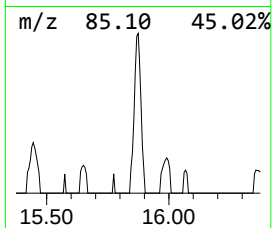
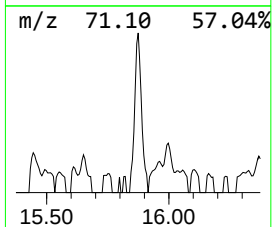
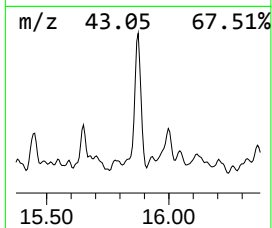
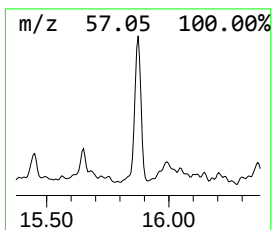
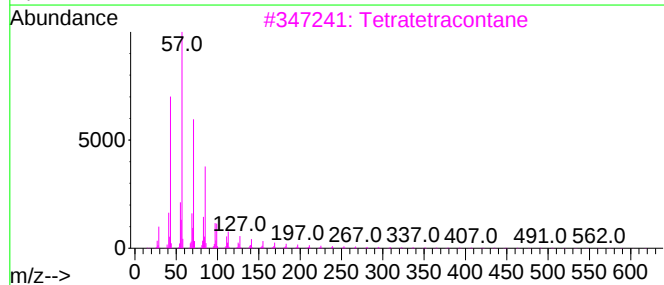
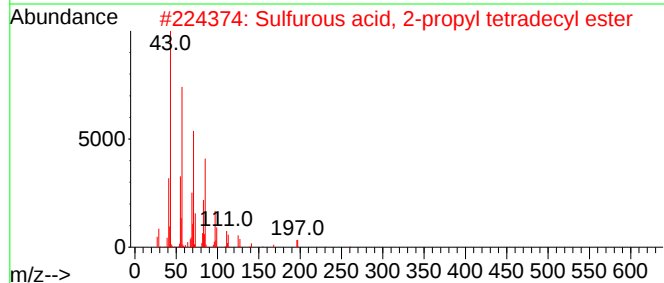
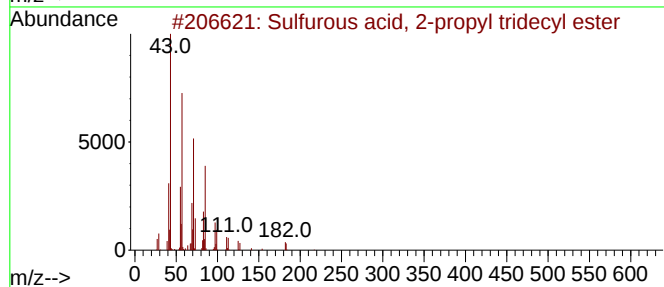
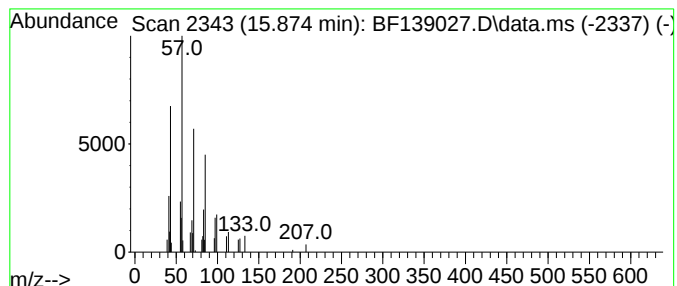
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Sulfurous acid, 2-propyl tr... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.874	2.74 ng	25869	Perylene-d12	15.462

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	87
2			Sulfurous acid, 2-propyl tetradec...	320	C17H36O3S	1010309-12-5	86
3			Tetratetracontane	619	C44H90	007098-22-8	86
4			Octacosane, 2-methyl-	408	C29H60	001560-98-1	80
5			Hentriacontane	437	C31H64	000630-04-6	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081524\
Data File : BF139027.D
Acq On : 15 Aug 2024 17:37
Operator : RC/JU
Sample : P3580-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
925-K1-SD-0-0.5-081224

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF073024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.057	4.6	ng	54287	1	6.834	235973	20.0
1-Phenoxypropan...	8.433	3.2	ng	48320	2	8.116	301959	20.0
Tridecane, 3-me...	10.769	2.1	ng	37541	4	11.357	350508	20.0
1-Decanol, 2-he...	13.827	5.0	ng	46886	5	13.998	187621	20.0
Octacosane	15.074	3.1	ng	29757	6	15.462	188955	20.0
Sulfurous acid,...	15.874	2.7	ng	25869	6	15.462	188955	20.0