

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061824\
 Data File : BF138223.D
 Acq On : 18 Jun 2024 14:31
 Operator : CG\JU
 Sample : P2918-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 POLE

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-BF061224.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138223.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.222	15	23	28	rBV	4497505	5751335	63.97%	8.788%
2	3.440	224	230	245	rBV	214474	408477	4.54%	0.624%
3	5.093	506	511	513	rBV	78978	94025	1.05%	0.144%
4	5.122	513	516	526	rVB	488563	563659	6.27%	0.861%
5	5.516	578	583	586	rBV	6684553	7403497	82.35%	11.312%
6	6.522	747	754	757	rBV	6623142	7395149	82.25%	11.299%
7	6.716	783	787	793	rBV	216368	201494	2.24%	0.308%
8	6.892	813	817	820	rBV	2822632	2155292	23.97%	3.293%
9	7.457	907	913	916	rBV	5075685	4843034	53.87%	7.400%
10	7.704	951	955	958	rBV	270107	196622	2.19%	0.300%
11	8.175	1030	1035	1038	rBV	3474205	2912707	32.40%	4.450%
12	8.481	1083	1087	1097	rBV	455349	422874	4.70%	0.646%
13	9.251	1212	1218	1221	rBV	9713496	8990701	100.00%	13.737%
14	9.928	1329	1333	1336	rBV	3399167	3080928	34.27%	4.707%
15	10.022	1344	1349	1363	rVB	1235370	1559823	17.35%	2.383%
16	10.710	1462	1466	1470	rBV	4875789	4413370	49.09%	6.743%
17	11.410	1581	1585	1588	rBV	2981885	2481529	27.60%	3.792%
18	11.933	1671	1674	1679	rBV2	426127	369711	4.11%	0.565%
19	12.622	1787	1791	1796	rVB	224857	209072	2.33%	0.319%
20	12.716	1804	1807	1815	rBV2	121711	143345	1.59%	0.219%
21	12.845	1822	1829	1832	rBV	211410	231022	2.57%	0.353%
22	12.998	1850	1855	1858	rBV	6845995	6387715	71.05%	9.760%
23	13.898	2004	2008	2017	rBV2	216992	392141	4.36%	0.599%
24	14.045	2026	2033	2036	rBV	2295475	2189264	24.35%	3.345%
25	14.068	2036	2037	2043	rVB	165411	107804	1.20%	0.165%
26	14.139	2045	2049	2056	rBV	143963	184458	2.05%	0.282%
27	14.516	2110	2113	2116	rBV	106158	97422	1.08%	0.149%
28	14.810	2159	2163	2165	rBV2	137287	176190	1.96%	0.269%
29	15.080	2205	2209	2212	rBV	123361	170083	1.89%	0.260%
30	15.110	2212	2214	2220	rVB	89188	95604	1.06%	0.146%
31	15.168	2220	2224	2231	rBV2	122410	156232	1.74%	0.239%
32	15.515	2278	2283	2288	rBV	1237428	1558092	17.33%	2.381%
33	16.004	2362	2366	2371	rBV	73111	106134	1.18%	0.162%

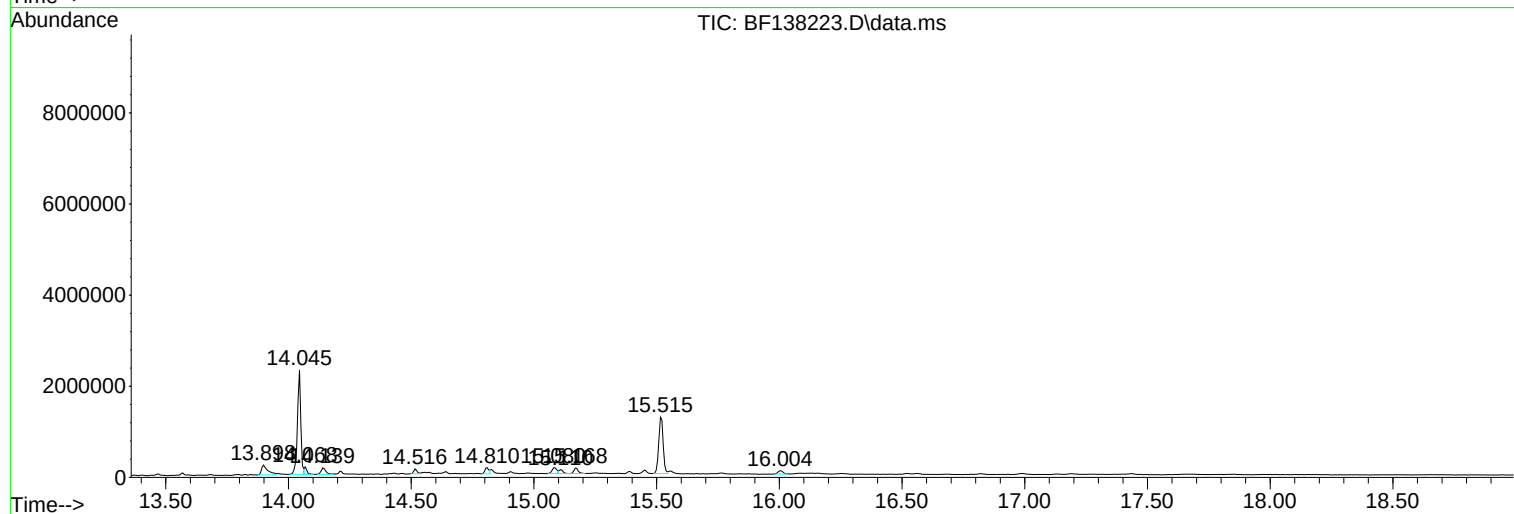
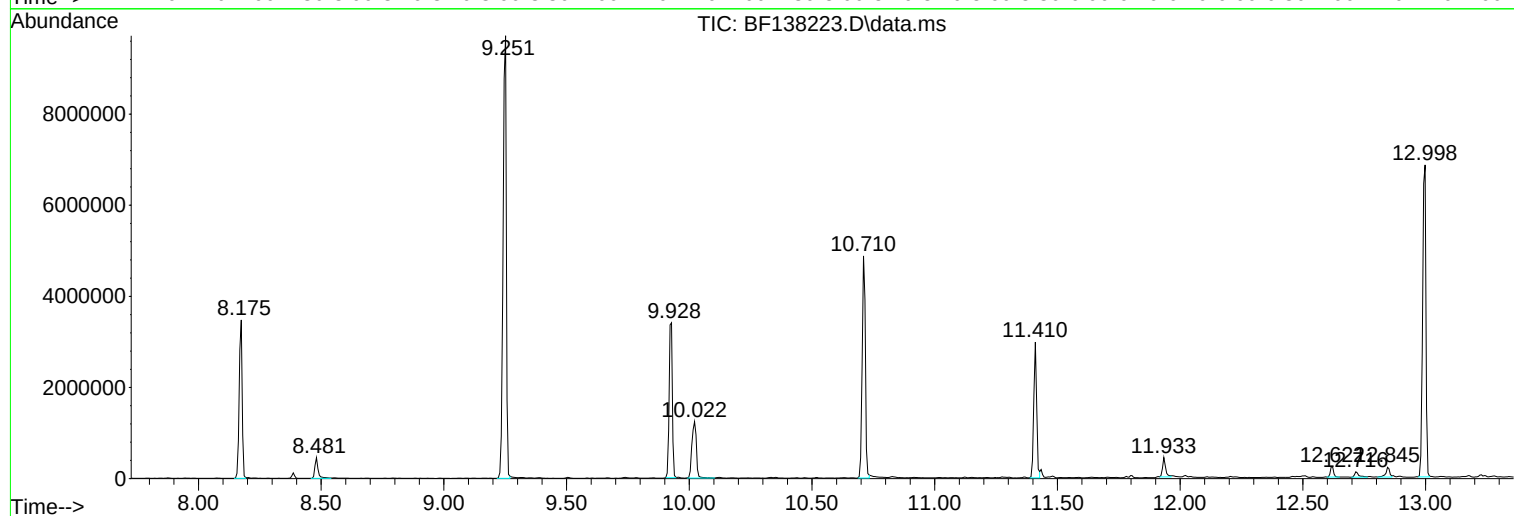
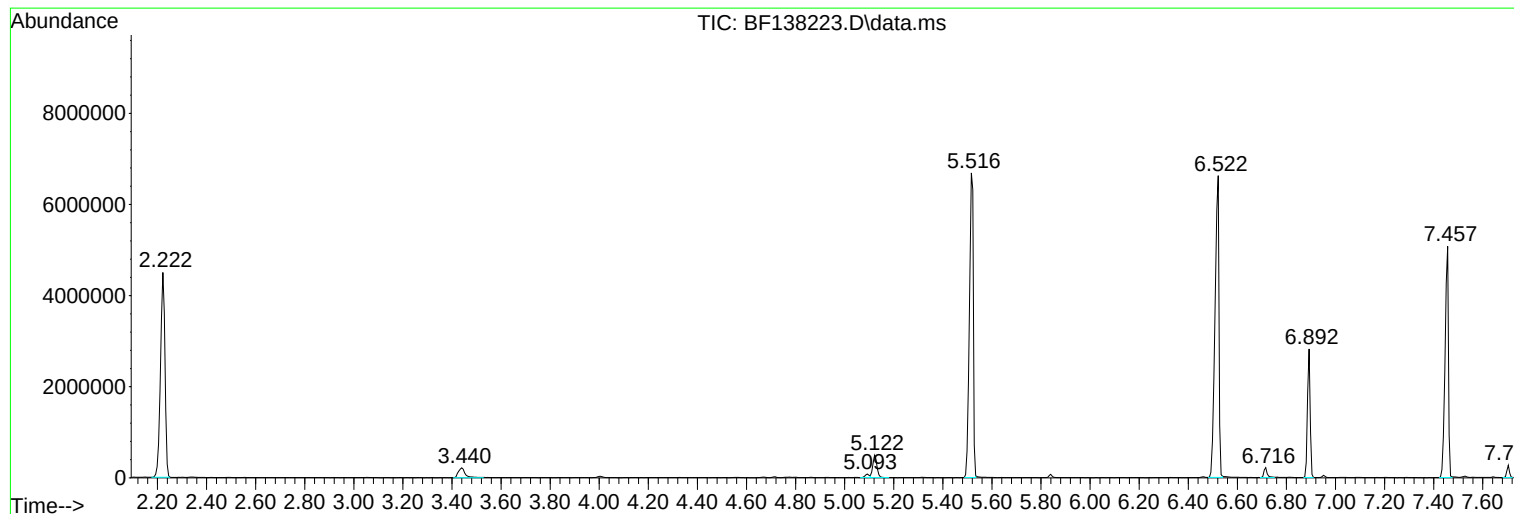
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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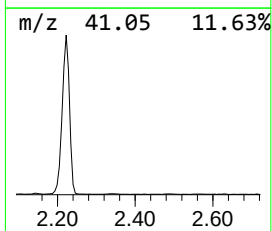
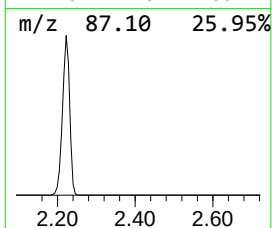
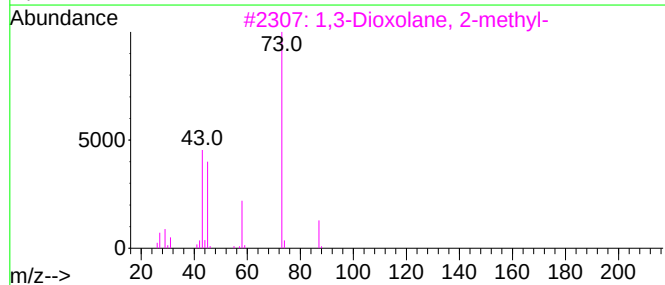
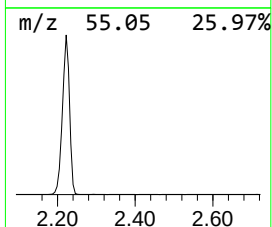
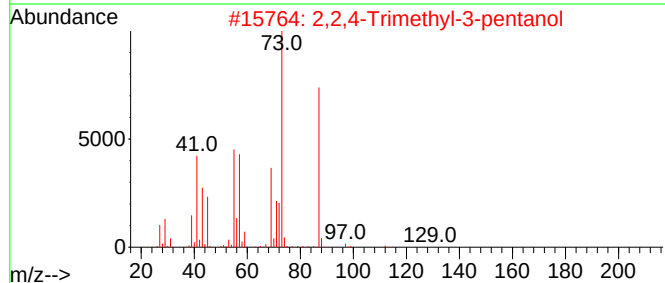
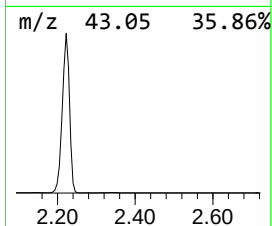
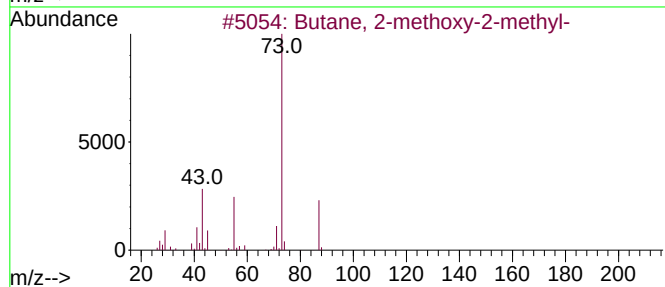
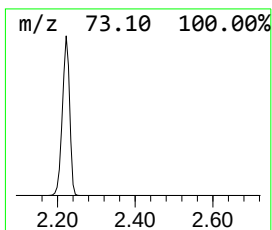
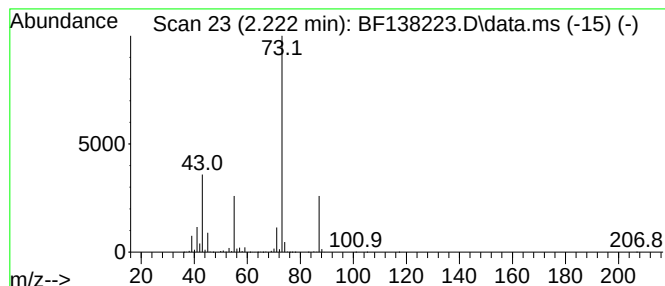
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.222	53.37 ng	5751340	1,4-Dichlorobenzene-d4	6.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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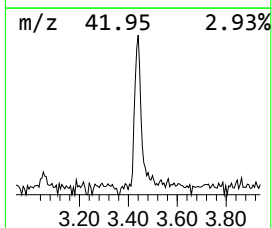
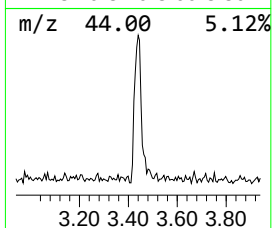
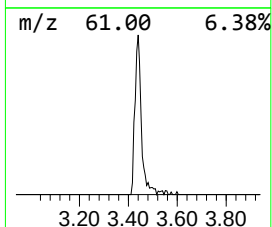
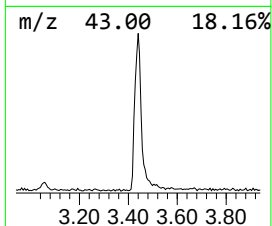
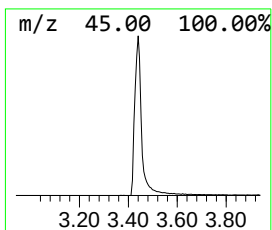
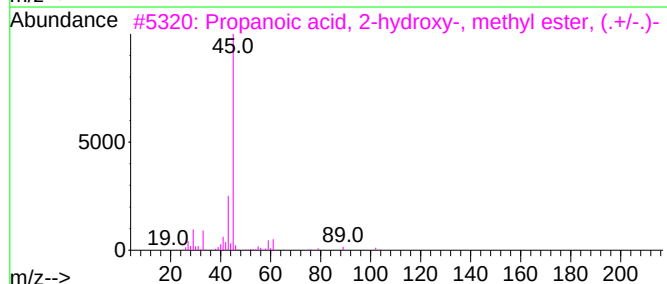
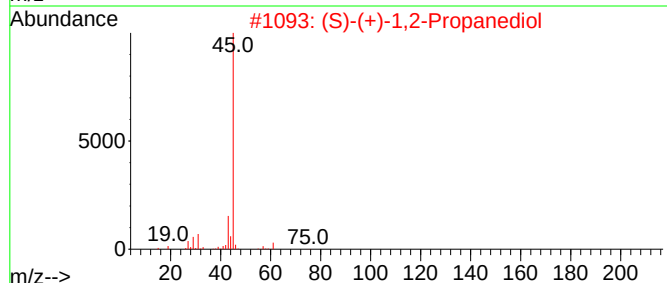
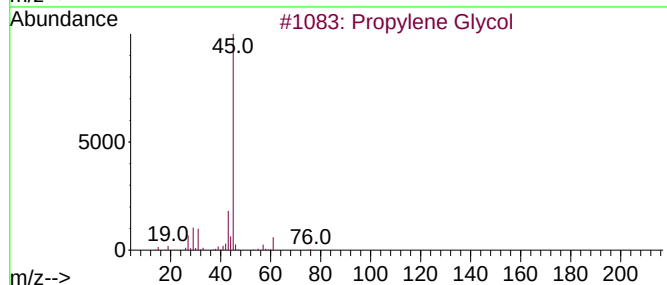
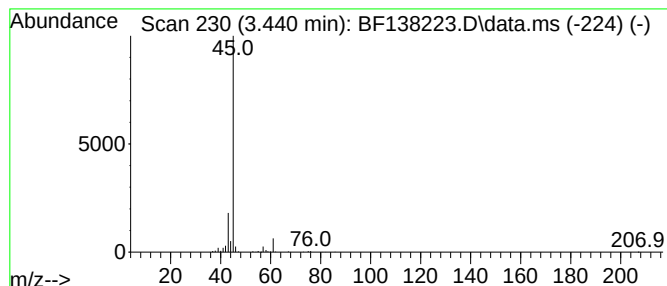
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Propylene Glycol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.440	3.79 ng	408477	1,4-Dichlorobenzene-d4	6.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	90
2			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	43
3			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
4			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	37
5			Formamide	45	CH3NO	000075-12-7	7



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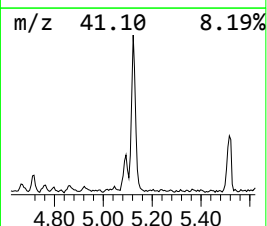
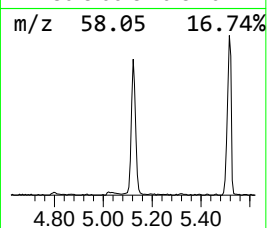
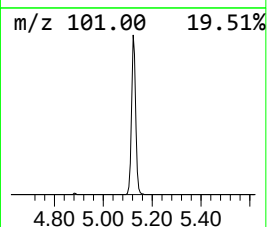
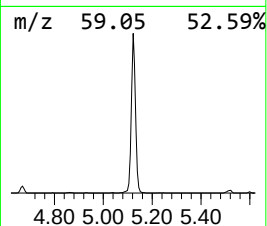
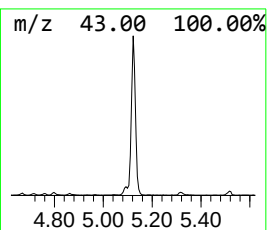
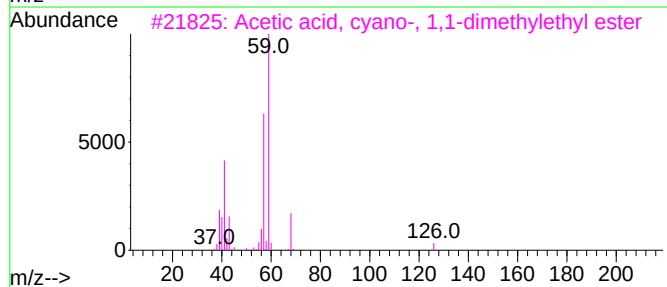
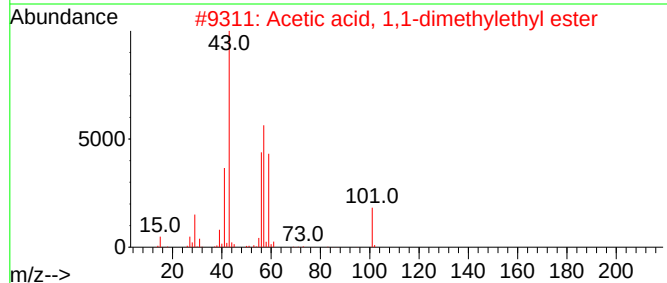
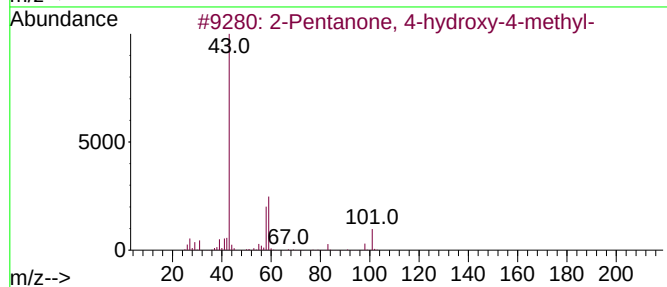
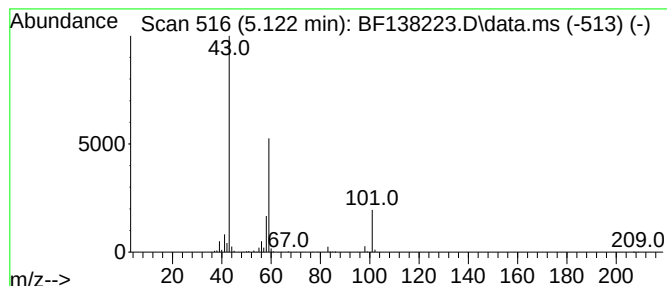
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.122	5.23 ng	563659	1,4-Dichlorobenzene-d4	6.892

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	39
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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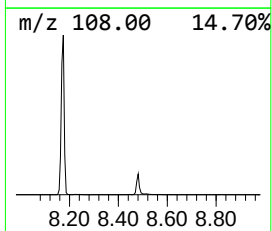
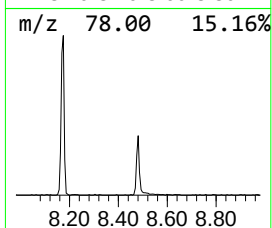
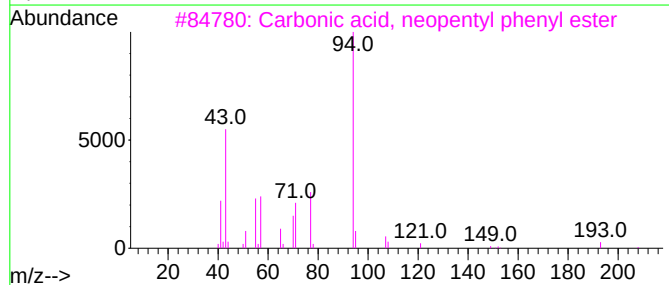
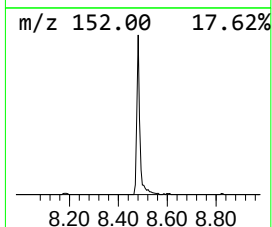
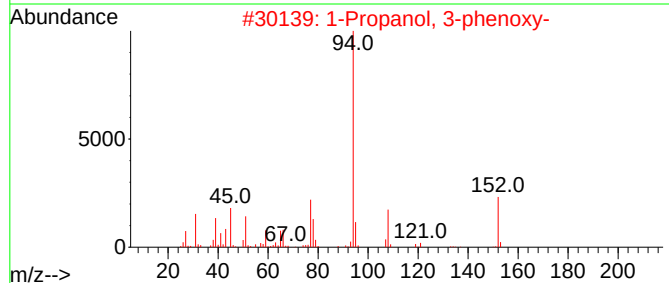
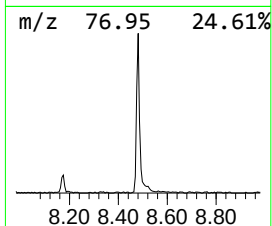
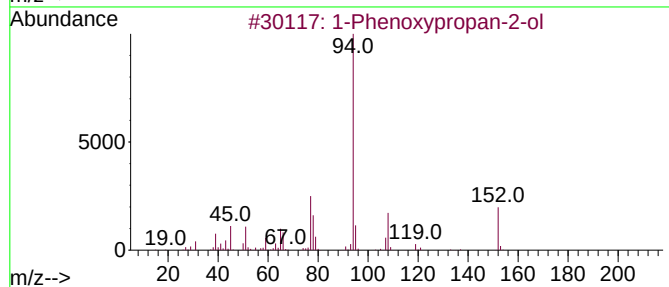
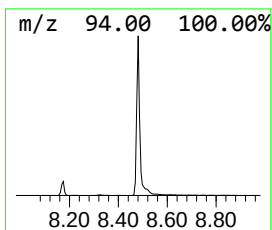
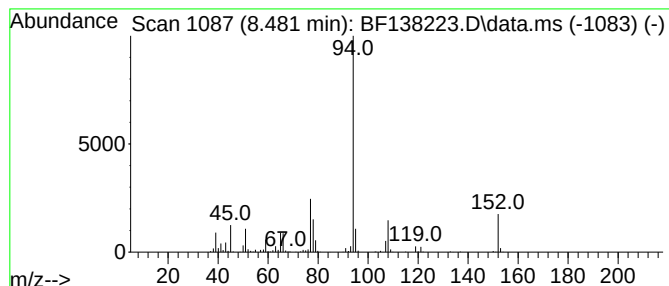
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Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.481	2.90 ng	422874	Naphthalene-d8	8.175

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	93
3		Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	64
4		1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
5		Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64



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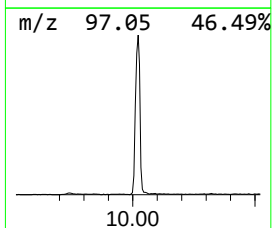
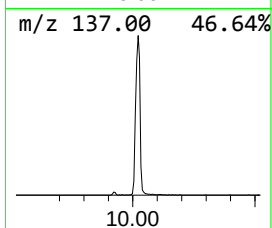
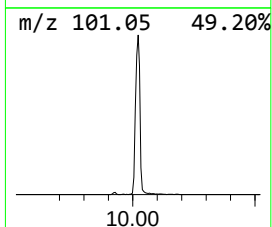
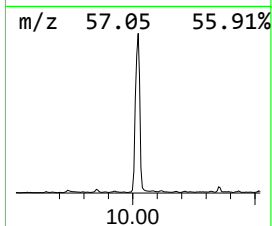
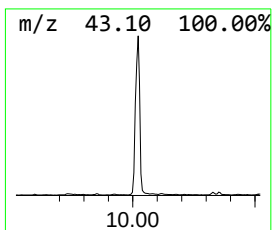
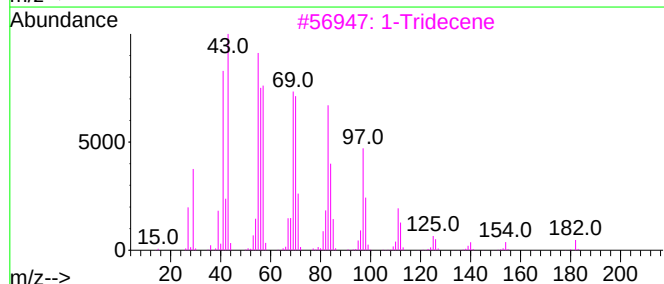
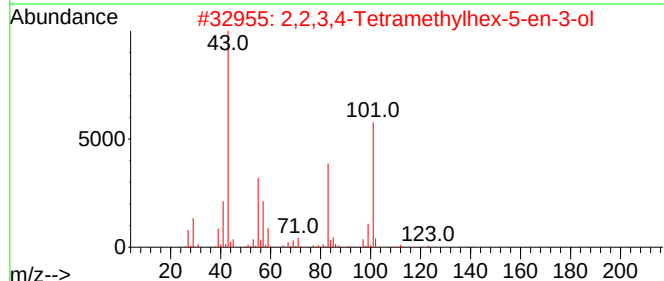
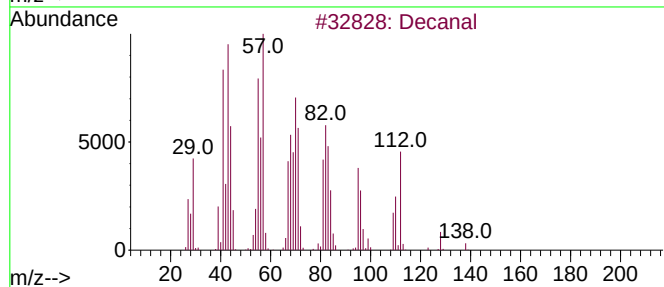
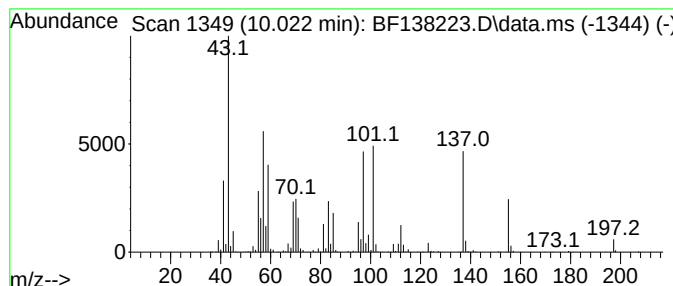
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 unknown10.022 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.022	10.13 ng	1559820	Acenaphthene-d10	9.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decanal	156	C10H20O	000112-31-2	10
2			2,2,3,4-Tetramethylhex-5-en-3-ol	156	C10H20O	1010191-06-9	10
3			1-Tridecene	182	C13H26	002437-56-1	10
4			trans-5-Isopropyl-6,7-epoxy-8-hy...	228	C13H24O3	058002-07-6	10
5			Carbonic acid, prop-1-en-2-yl un...	256	C15H28O3	1000382-90-6	10



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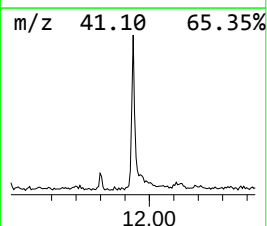
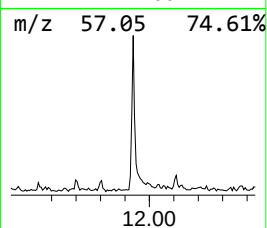
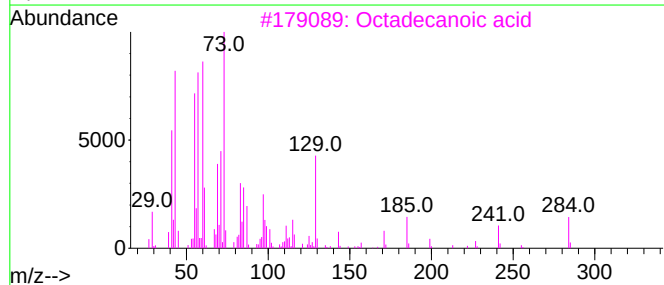
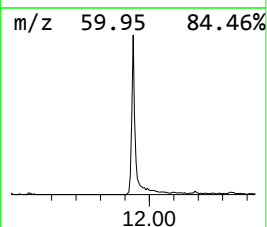
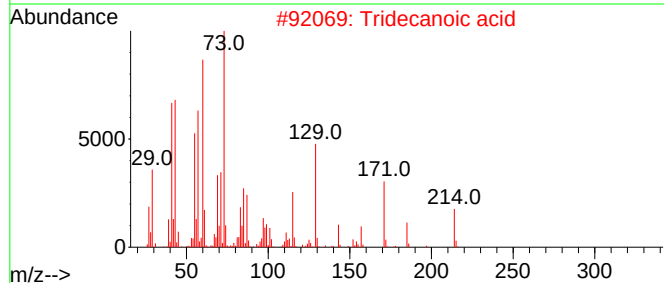
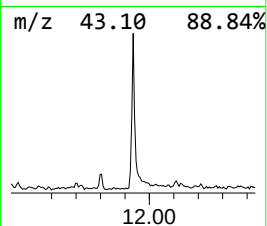
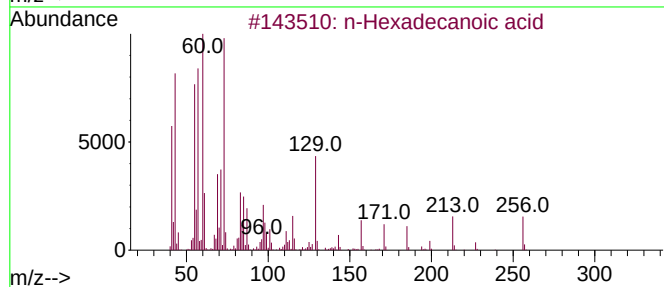
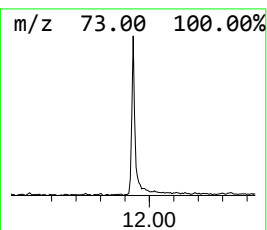
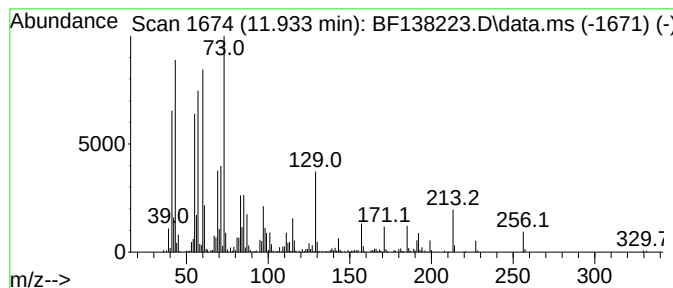
Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.933	2.98 ng	369711	Phenanthrene-d10		11.410	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Tridecanoic acid		214	C13H26O2	000638-53-9	93
3	Octadecanoic acid		284	C18H36O2	000057-11-4	93
4	Pentadecanoic acid		242	C15H30O2	001002-84-2	91
5	Tetradecanoic acid		228	C14H28O2	000544-63-8	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061824\
Data File : BF138223.D
Acq On : 18 Jun 2024 14:31
Operator : CG\JU
Sample : P2918-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

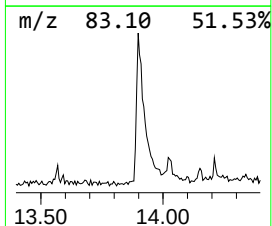
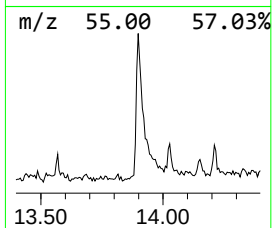
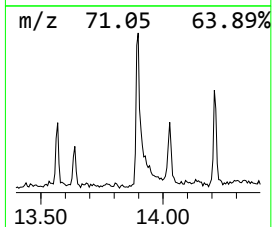
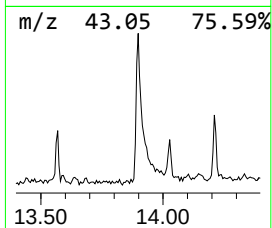
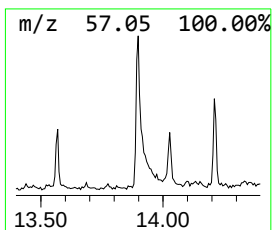
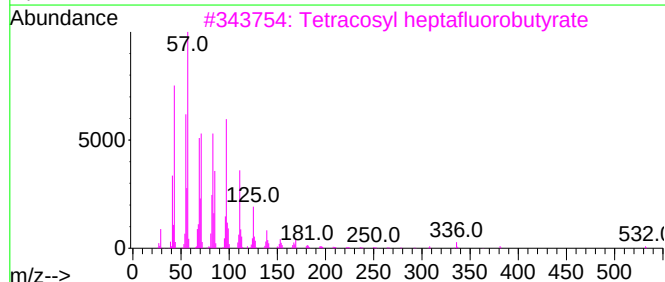
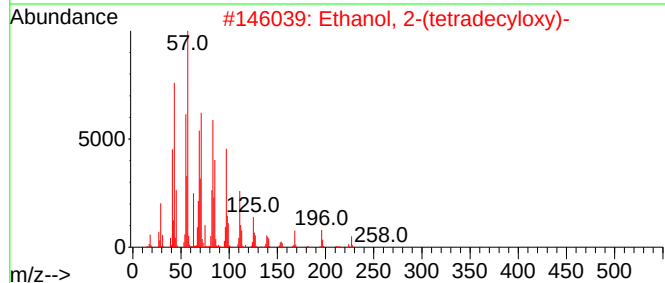
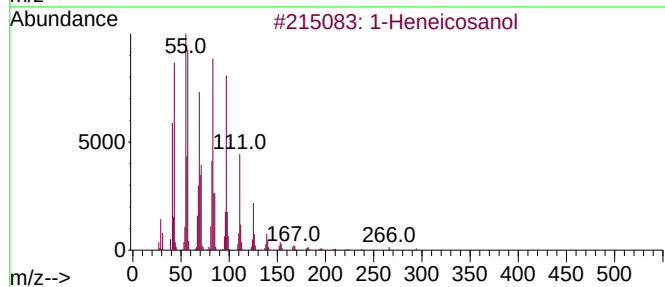
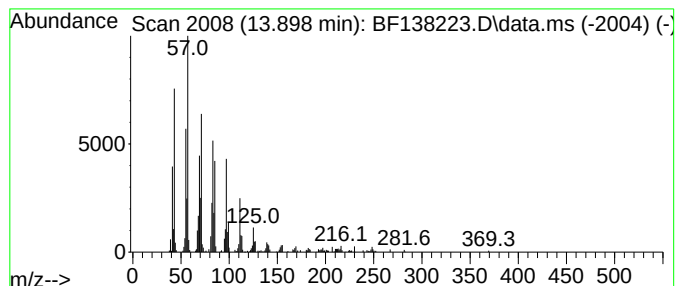
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.898	3.58 ng	392141	Chrysene-d12	14.045	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	92
2	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
3	Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	90
4	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	90
5	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061824\
Data File : BF138223.D
Acq On : 18 Jun 2024 14:31
Operator : CG\JU
Sample : P2918-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
POLE

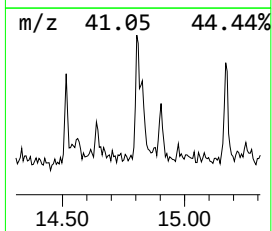
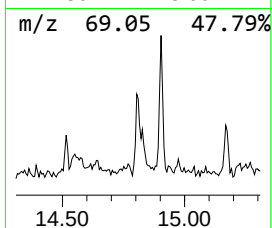
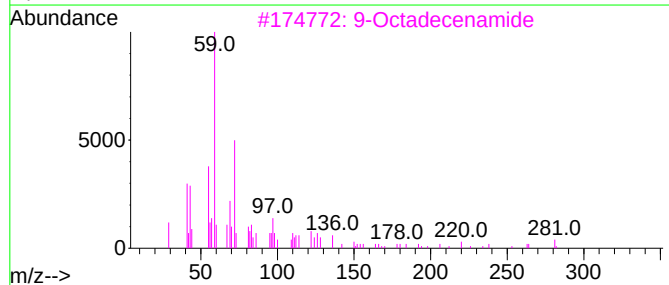
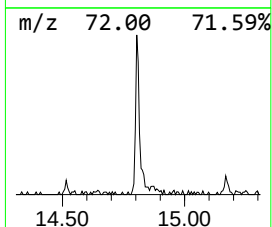
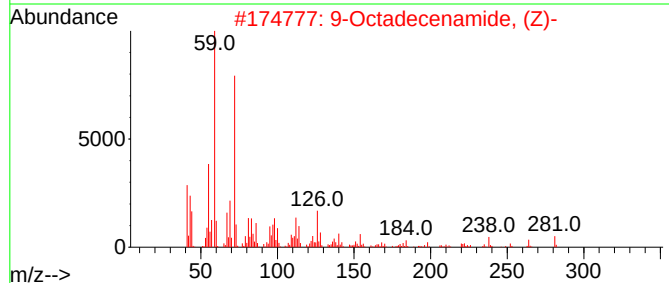
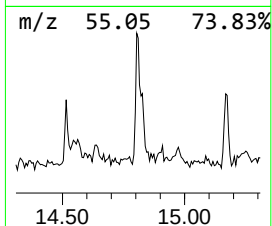
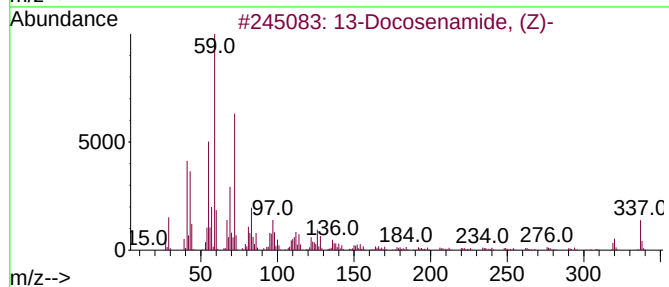
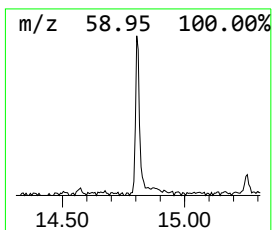
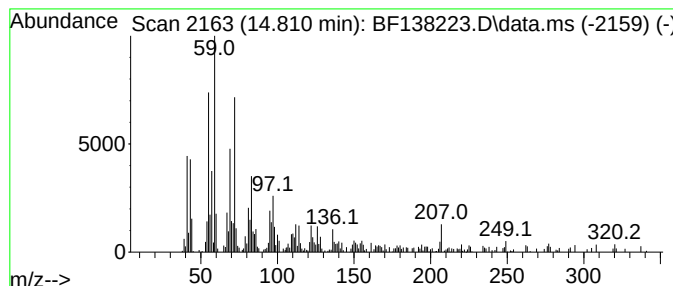
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 13-Docosenamide, (Z)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.810	2.26 ng	176190	Perylene-d12	15.521

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	89
2		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	64
3		9-Octadecenamide	281	C18H35NO	003322-62-1	58
4		7-Nonenamide	155	C9H17NO	090949-53-4	53
5		d,l-trans-4-Methyl-5-methoxy-1-(...	184	C11H20O2	1000101-22-2	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061824\
Data File : BF138223.D
Acq On : 18 Jun 2024 14:31
Operator : CG\JU
Sample : P2918-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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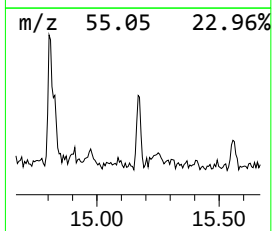
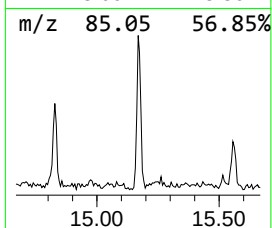
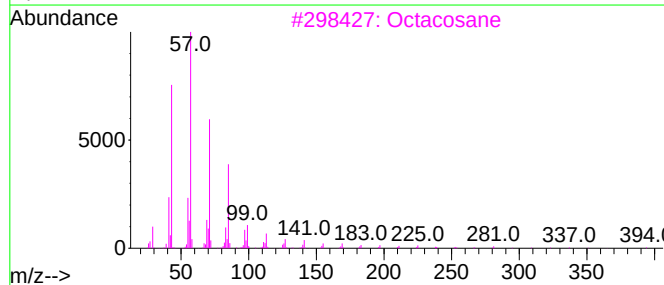
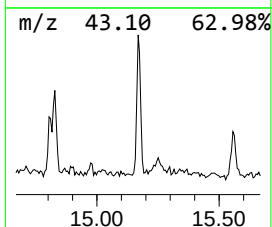
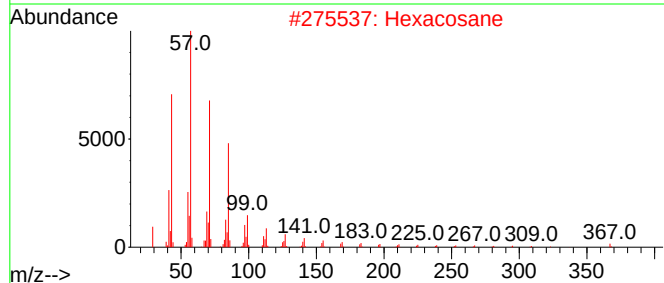
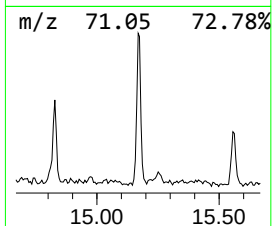
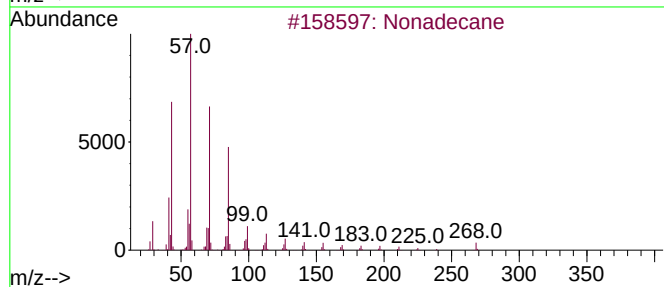
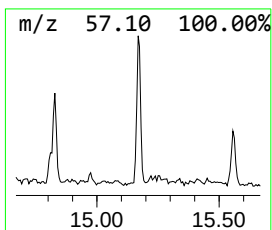
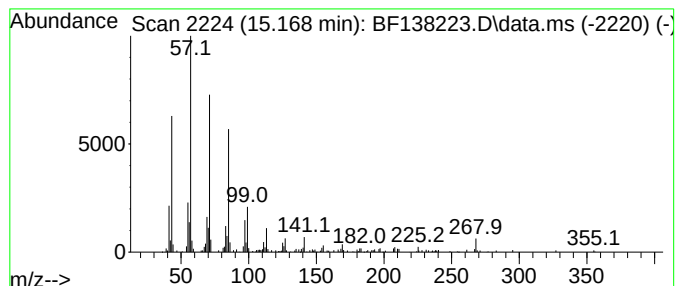
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Nonadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.168	2.01 ng	156232	Perylene-d12	15.521

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Nonadecane	268	C19H40	000629-92-5	90
2		Hexacosane	366	C26H54	000630-01-3	87
3		Octacosane	394	C28H58	000630-02-4	87
4		Triacontane	422	C30H62	000638-68-6	86
5		Heneicosane	296	C21H44	000629-94-7	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061824\
Data File : BF138223.D
Acq On : 18 Jun 2024 14:31
Operator : CG\JU
Sample : P2918-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
POLE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.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...	2.222	53.4	ng	5751340	1	6.892	2155290	20.0
Propylene Glycol	3.440	3.8	ng	408477	1	6.892	2155290	20.0
2-Pentanone, 4-...	5.122	5.2	ng	563659	1	6.892	2155290	20.0
1-Phenoxypropan...	8.481	2.9	ng	422874	2	8.175	2912710	20.0
unknown10.022	10.022	10.1	ng	1559820	3	9.928	3080930	20.0
n-Hexadecanoic ...	11.933	3.0	ng	369711	4	11.410	2481530	20.0
1-Heneicosanol	13.898	3.6	ng	392141	5	14.045	2189260	20.0
13-Docosenamide...	14.810	2.3	ng	176190	6	15.521	1558090	20.0
Nonadecane	15.168	2.0	ng	156232	6	15.521	1558090	20.0