

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083023\
 Data File : BF135012.D
 Acq On : 30 Aug 2023 19:07
 Operator : CG\JU
 Sample : 04152-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMPOSITE-1

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-BF083023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135012.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	3	8	23	rVB3	36591	101525	2.88%	0.450%
2	4.987	489	493	498	rVB	599019	634362	18.01%	2.813%
3	5.399	559	563	574	rVB	1328359	1140228	32.37%	5.056%
4	6.404	730	734	746	rBV	744628	718106	20.39%	3.184%
5	6.575	760	763	766	rBV	335229	273159	7.75%	1.211%
6	6.604	766	768	772	rVB	194055	148099	4.20%	0.657%
7	6.704	780	785	788	rBV	1180772	1115104	31.66%	4.945%
8	6.769	793	796	799	rBV	1160329	963408	27.35%	4.272%
9	6.804	799	802	805	rVB	902221	710708	20.18%	3.151%
10	7.175	862	865	868	rBV	103025	83187	2.36%	0.369%
11	7.334	887	892	895	rBV	2117453	2115302	60.05%	9.380%
12	8.051	1009	1014	1017	rBV	1458469	1269433	36.04%	5.629%
13	8.598	1101	1107	1112	rBV2	35912	39262	1.11%	0.174%
14	9.134	1192	1198	1201	rBV	3597989	3522420	100.00%	15.619%
15	9.251	1213	1218	1222	rVB3	48411	49128	1.39%	0.218%
16	9.434	1245	1249	1251	rBV	114658	102242	2.90%	0.453%
17	9.681	1285	1291	1294	rBV2	32818	44503	1.26%	0.197%
18	9.810	1308	1313	1316	rBV	1382993	1292134	36.68%	5.730%
19	10.016	1340	1348	1350	rBV8	19902	37614	1.07%	0.167%
20	10.234	1381	1385	1388	rVB	211224	169442	4.81%	0.751%
21	10.310	1394	1398	1403	rVB5	45999	48008	1.36%	0.213%
22	10.598	1443	1447	1451	rBV	1571066	1324099	37.59%	5.871%
23	10.816	1482	1484	1488	rVB2	31460	35547	1.01%	0.158%
24	10.969	1506	1510	1513	rVB2	62186	74302	2.11%	0.329%
25	11.298	1562	1566	1570	rVB	1239717	1070771	30.40%	4.748%
26	11.839	1652	1658	1668	rBV2	679637	872954	24.78%	3.871%
27	12.633	1787	1793	1804	rBV	516991	586334	16.65%	2.600%
28	12.898	1834	1838	1841	rBV	2322451	2051826	58.25%	9.098%
29	13.816	1991	1994	2002	rVB	113989	132221	3.75%	0.586%
30	13.957	2014	2018	2022	rBV	936200	805172	22.86%	3.570%
31	15.427	2263	2268	2275	rBV	712999	841670	23.89%	3.732%
32	16.574	2459	2463	2470	rVB2	107609	179234	5.09%	0.795%

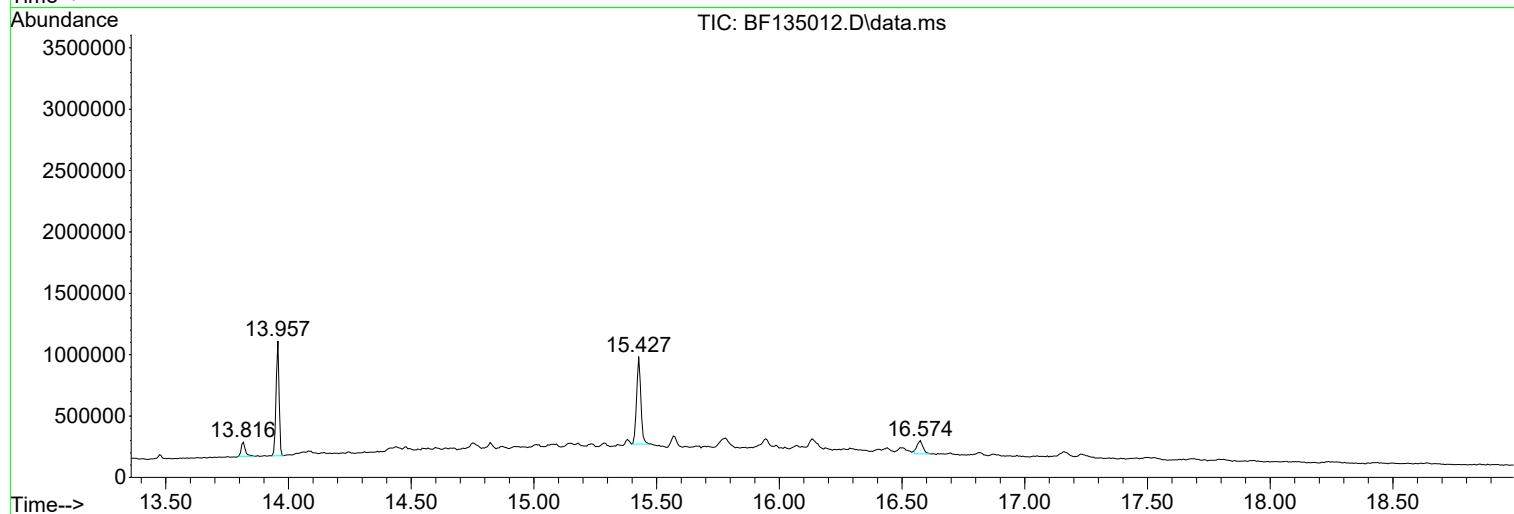
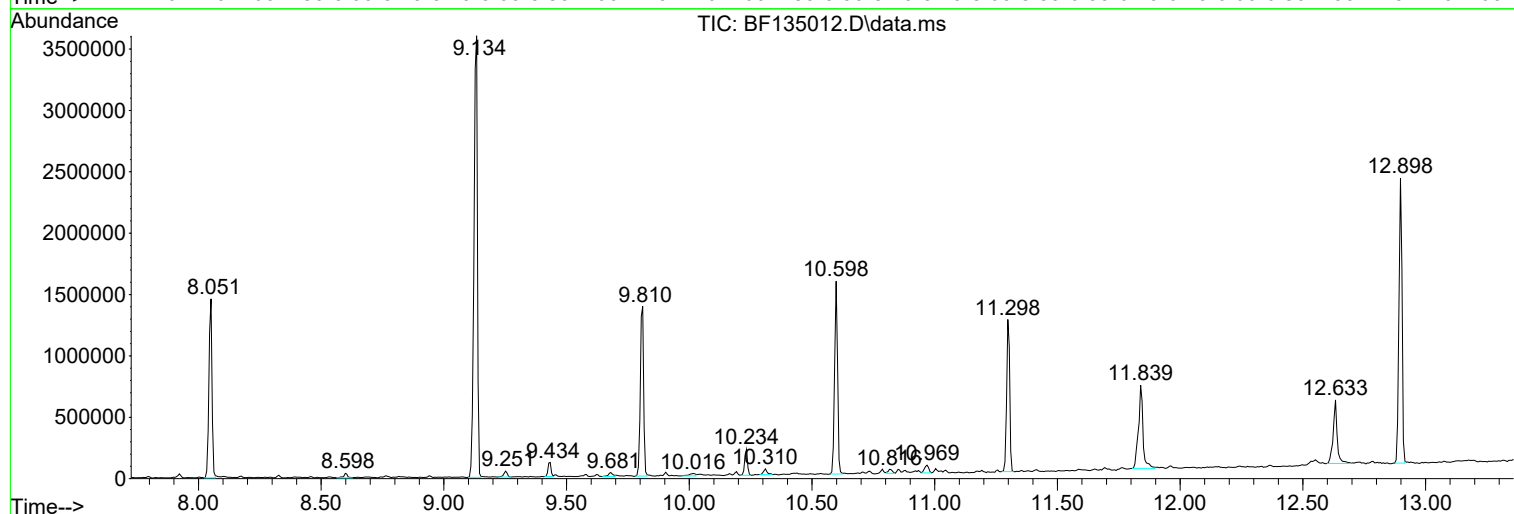
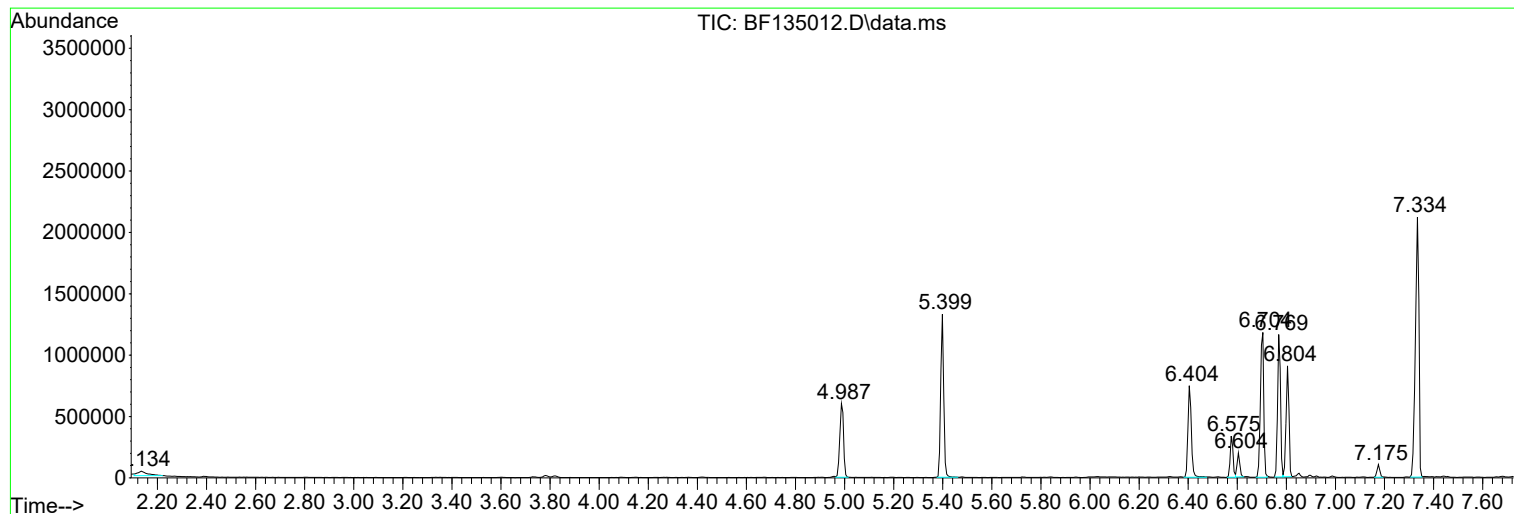
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Operator : CG\JU
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Instrument :
BNA_F
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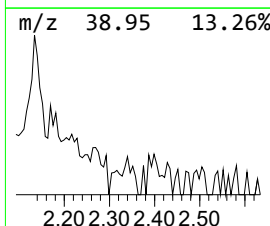
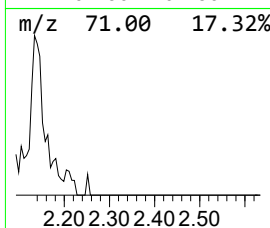
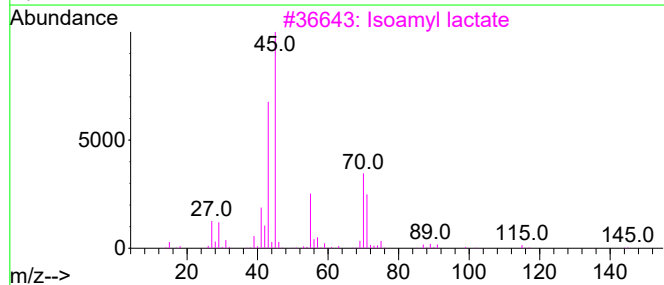
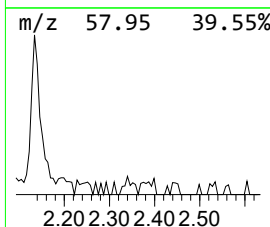
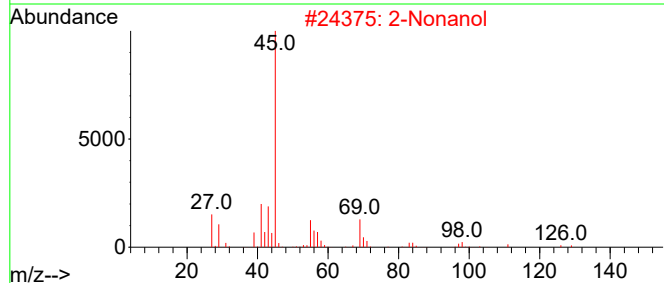
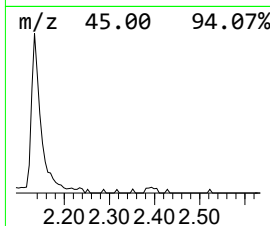
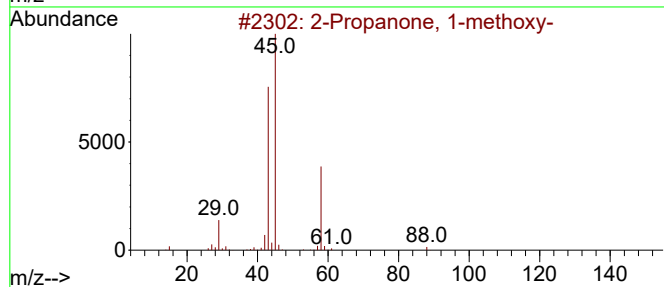
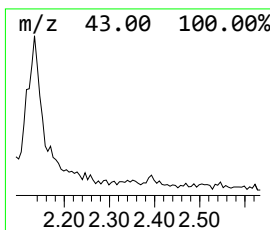
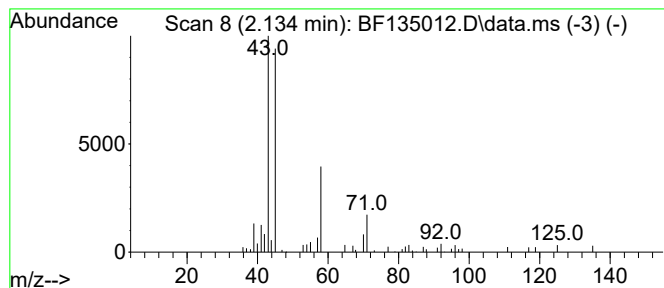
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown2.134 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.134	2.11 ng	101525	1,4-Dichlorobenzene-d4	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanone, 1-methoxy-			88	C4H8O2	005878-19-3	45
2	2-Nonanol			144	C9H20O	000628-99-9	32
3	Isoamyl lactate			160	C8H16O3	019329-89-6	28
4	2-Hexadecanol			242	C16H34O	014852-31-4	25
5	1-Pentanol, 5-methoxy-			118	C6H14O2	004799-62-6	25



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ClientSampleId :
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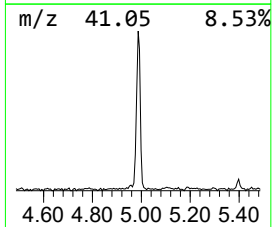
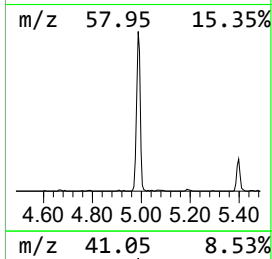
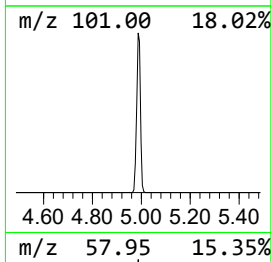
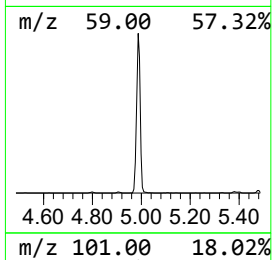
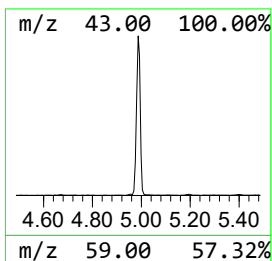
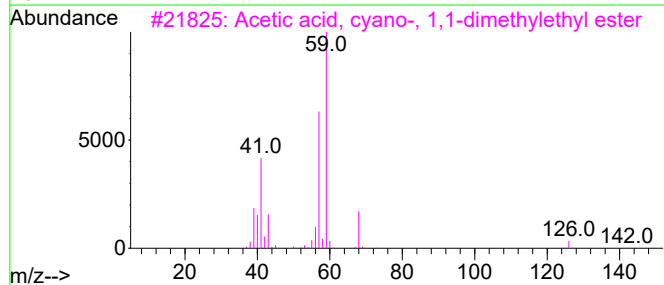
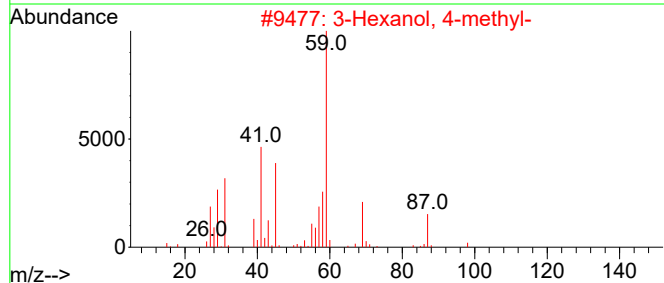
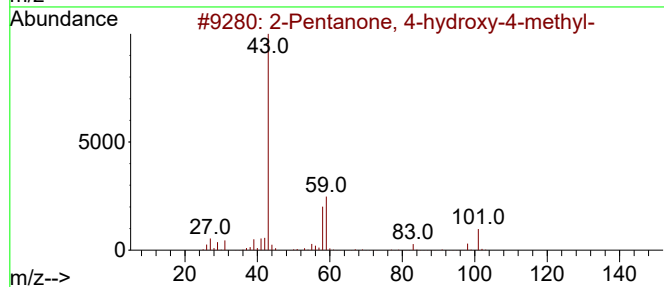
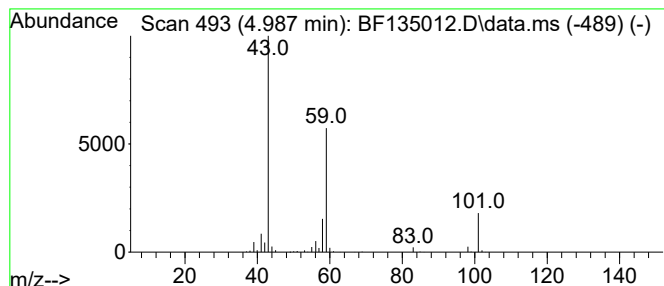
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.987	13.17 ng	634362	1,4-Dichlorobenzene-d4	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		
5	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9		



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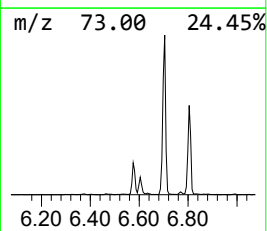
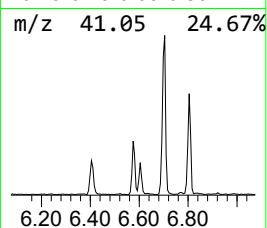
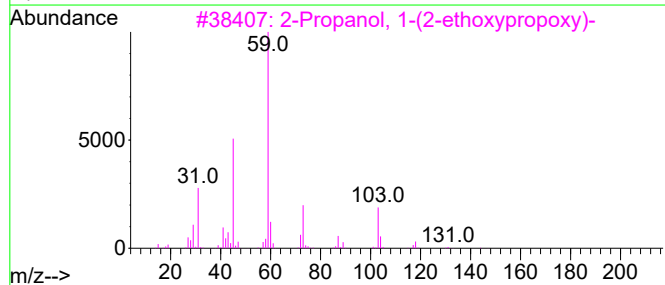
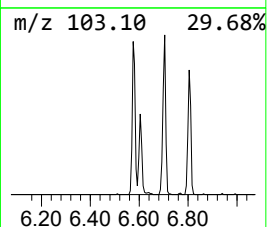
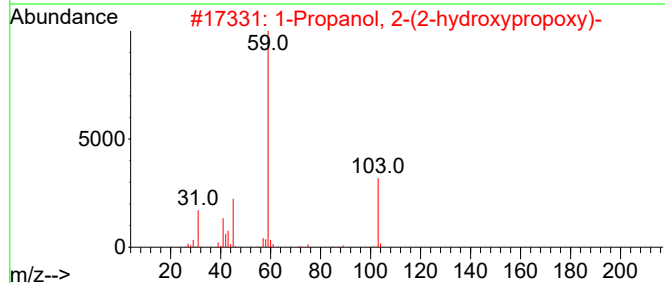
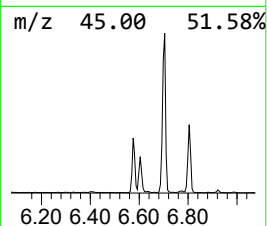
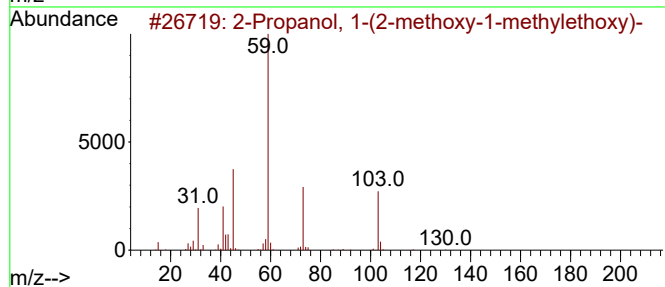
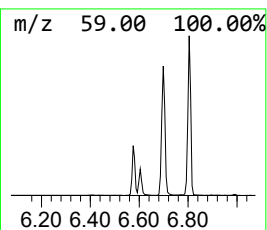
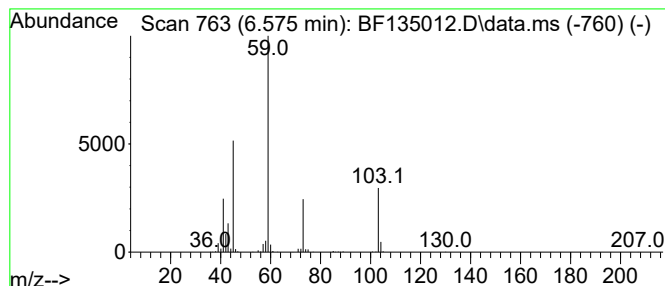
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Propanol, 1-(2-methoxy-1-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.575	5.67 ng	273159	1,4-Dichlorobenzene-d4	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	72		
2	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	59		
3	2-Propanol, 1-(2-ethoxypropoxy)-	162	C8H18O3	010143-32-5	56		
4	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	50		
5	Ethane, 1-ethoxy-1-methoxy-	104	C5H12O2	010471-14-4	50		



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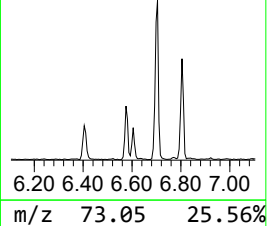
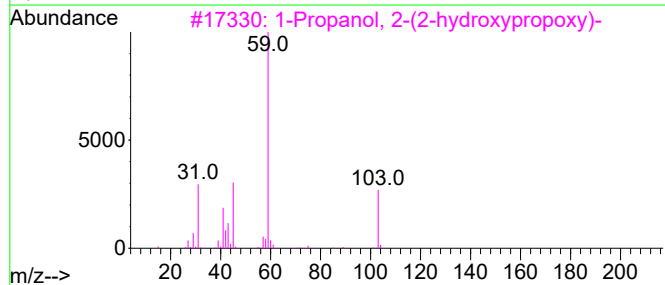
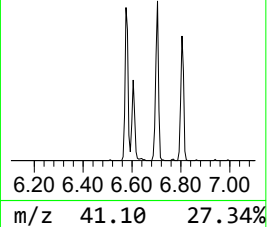
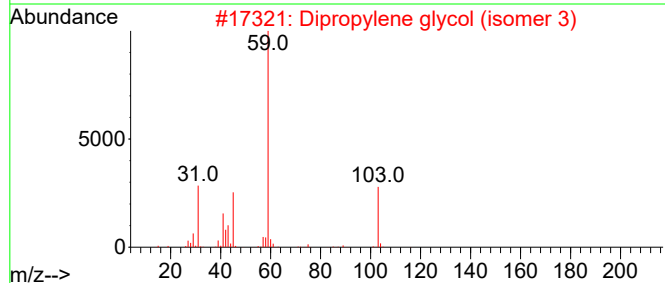
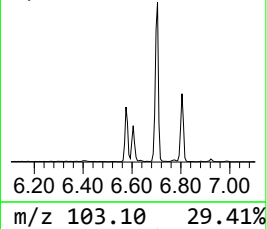
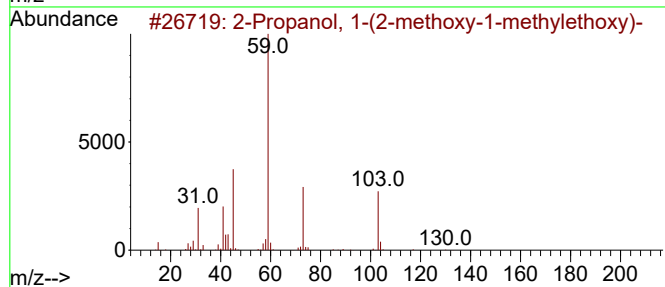
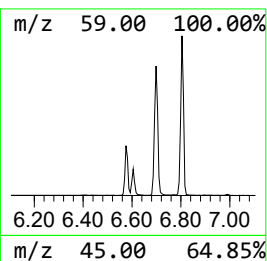
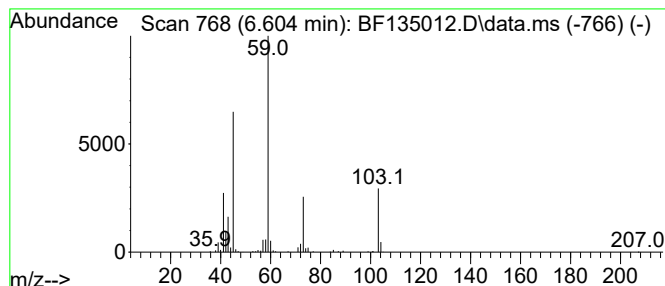
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Dipropylene glycol (isomer 3) Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.604	3.07 ng	148099	1,4-Dichlorobenzene-d4	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	72		
2	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	53		
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	53		
4	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	53		
5	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	53		



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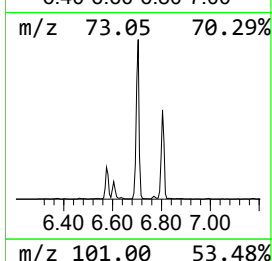
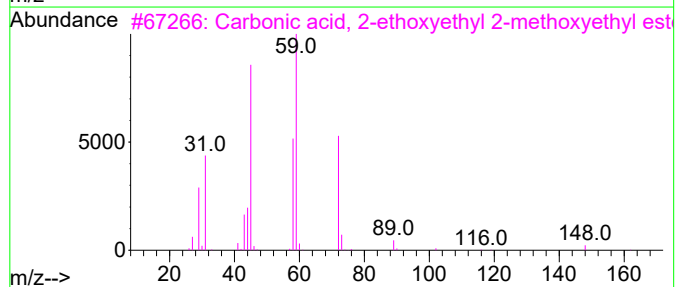
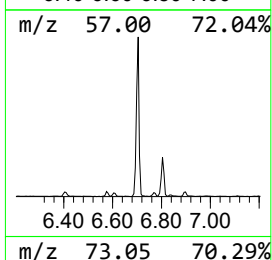
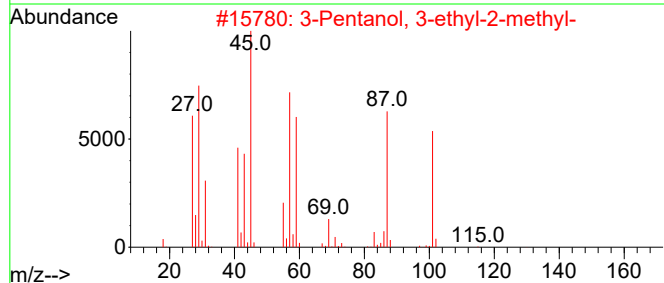
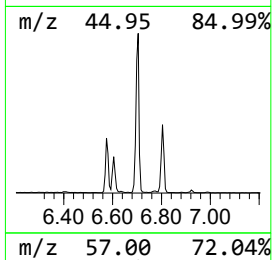
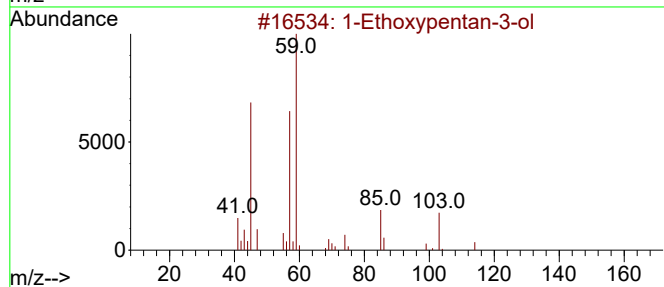
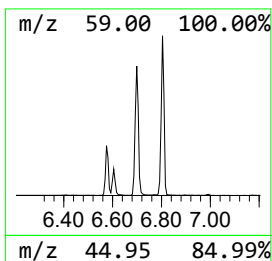
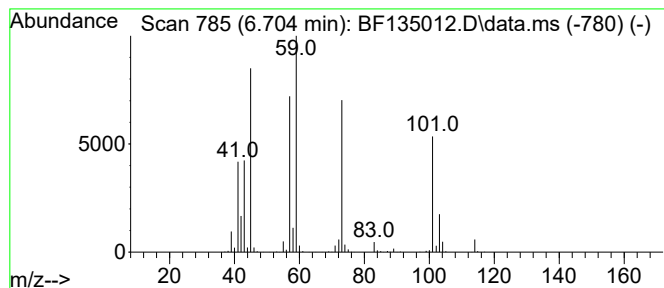
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown6.704 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.704	23.15 ng	1115100	1,4-Dichlorobenzene-d4	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Ethoxypentan-3-ol	132	C7H16O2	100910-92-7	45
2			3-Pentanol, 3-ethyl-2-methyl-	130	C8H18O	000597-05-7	40
3			Carbonic acid, 2-ethoxyethyl 2-m...	192	C8H16O5	1000331-46-1	40
4			Di-sec-Butyl ether	130	C8H18O	006863-58-7	38
5			Sulfurous acid, isobutyl 2-methy...	238	C10H22O4S	1000309-20-3	37



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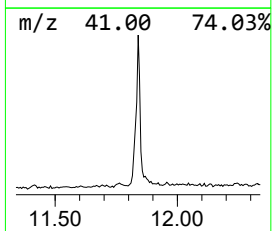
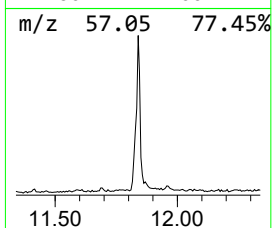
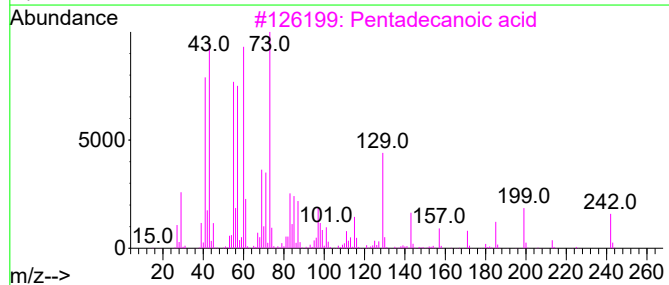
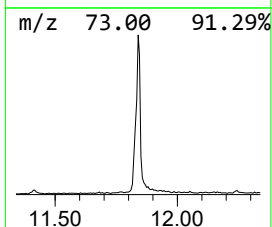
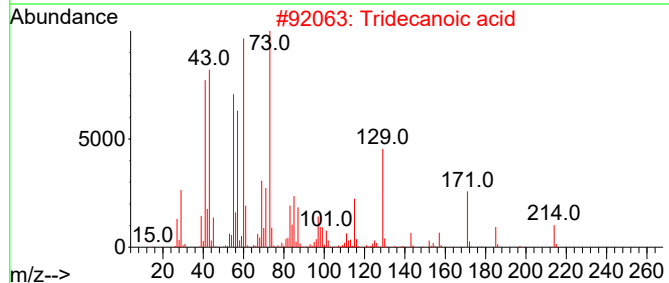
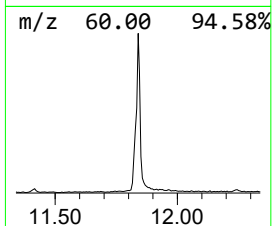
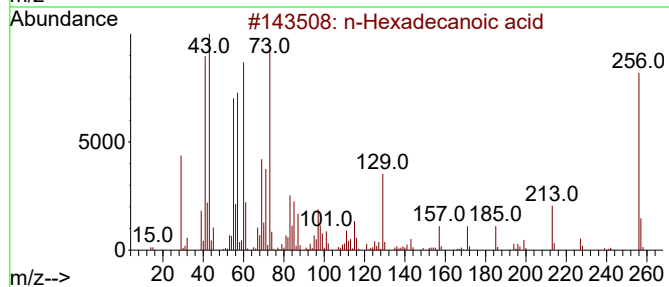
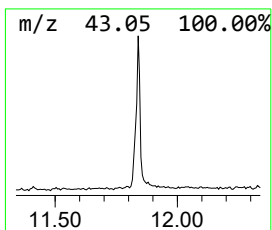
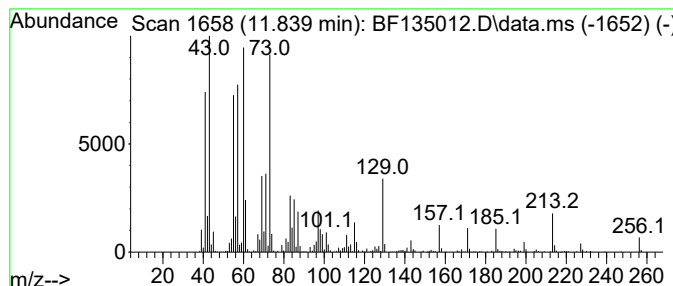
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	16.31 ng	872954	Phenanthrene-d10	11.298

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	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			Dodecanoic acid	200	C12H24O2	000143-07-7	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083023\
Data File : BF135012.D
Acq On : 30 Aug 2023 19:07
Operator : CG\JU
Sample : 04152-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSITE-1

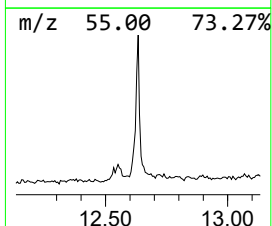
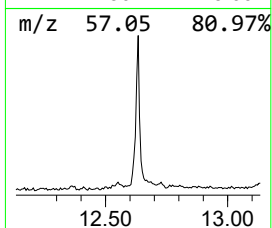
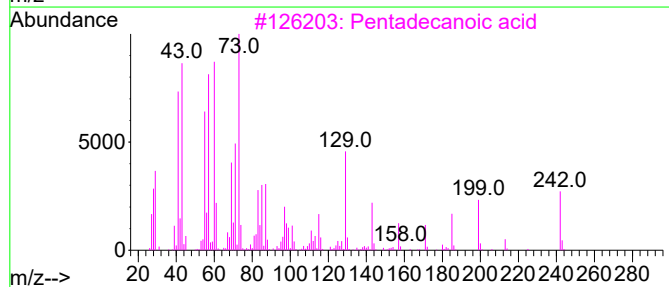
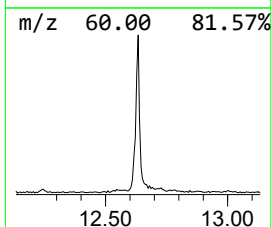
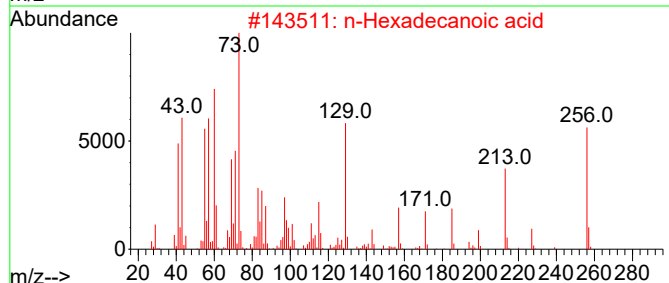
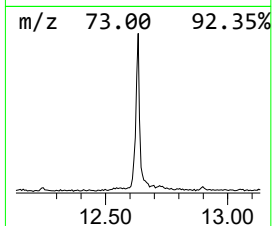
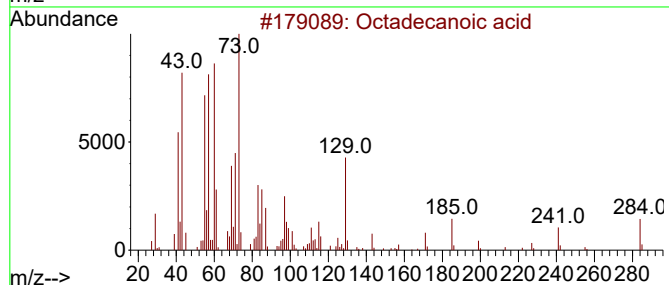
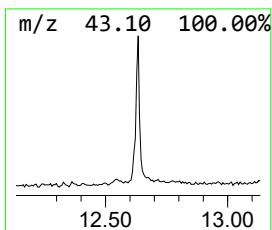
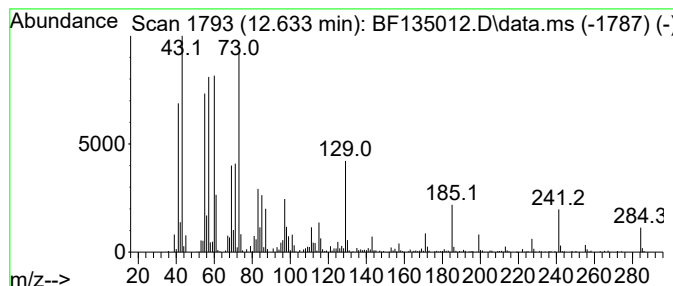
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.633	14.56 ng	586334	Chrysene-d12	13.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			n-Decanoic acid	172	C10H20O2	000334-48-5	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083023\
Data File : BF135012.D
Acq On : 30 Aug 2023 19:07
Operator : CG\JU
Sample : 04152-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSITE-1

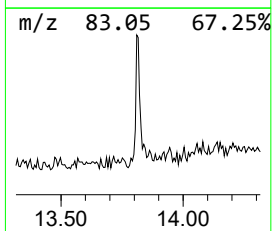
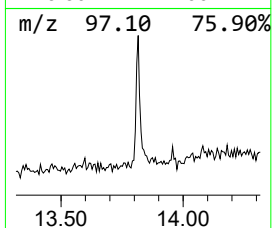
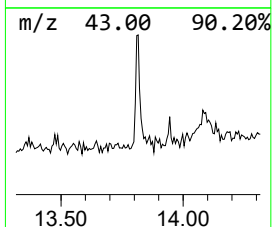
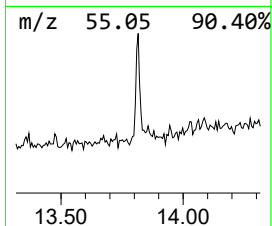
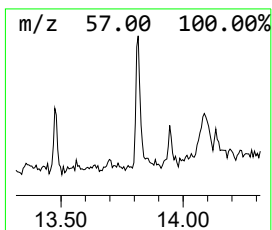
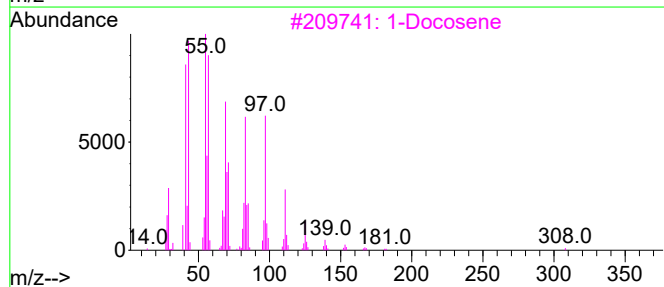
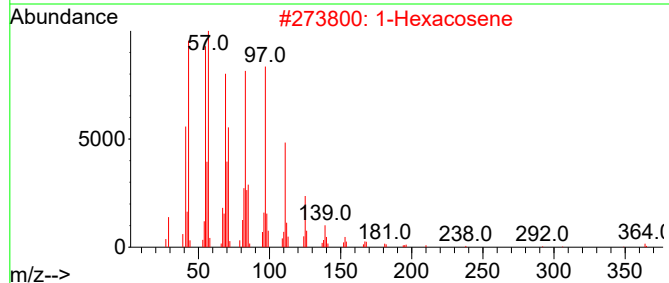
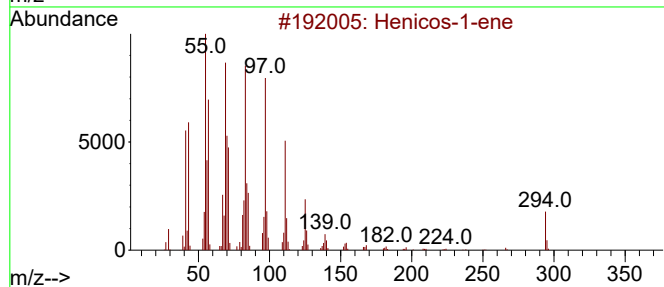
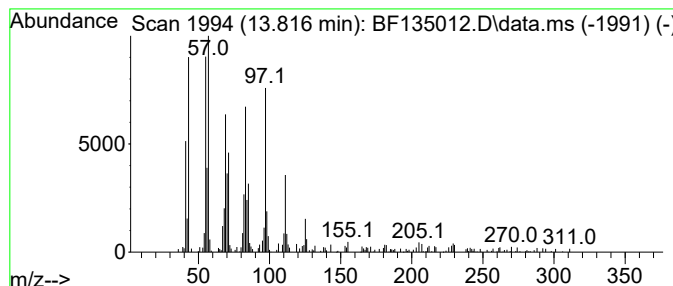
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Henicos-1-ene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.816	3.28 ng	132221	Chrysene-d12	13.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Henicos-1-ene	294	C21H42	001599-68-4	94
2			1-Hexacosene	364	C26H52	018835-33-1	91
3			1-Docosene	308	C22H44	001599-67-3	91
4			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	91
5			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083023\
Data File : BF135012.D
Acq On : 30 Aug 2023 19:07
Operator : CG\JU
Sample : 04152-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSITE-1

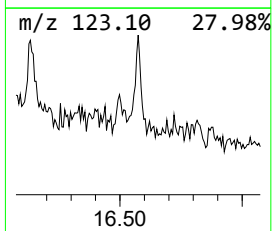
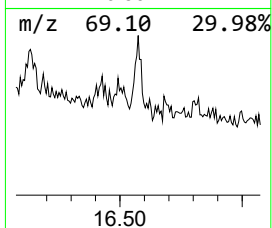
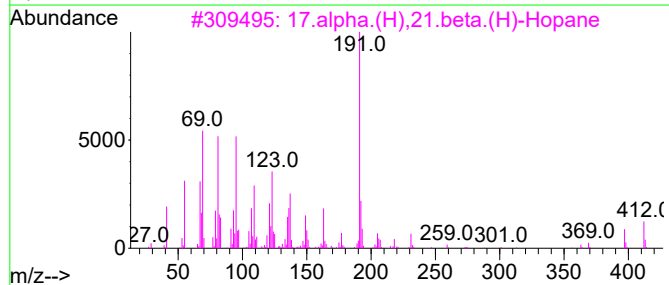
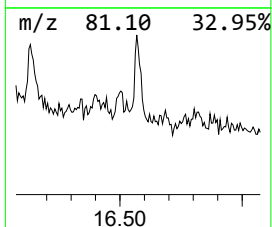
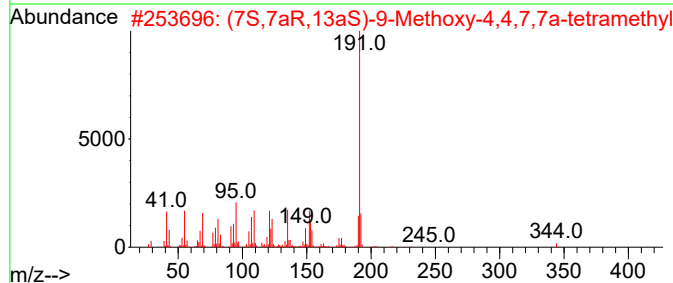
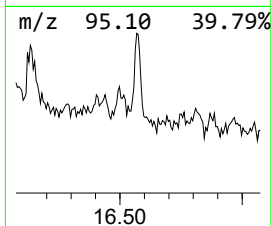
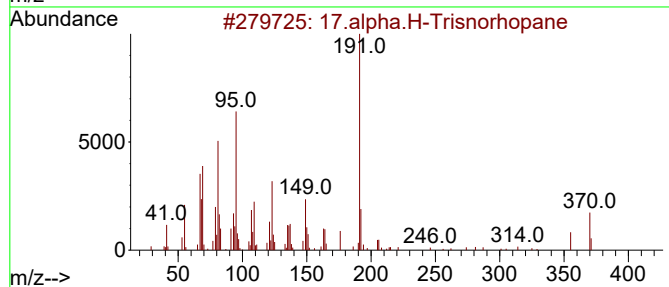
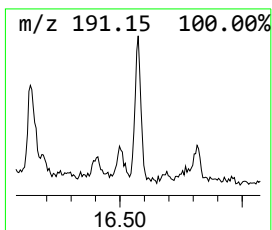
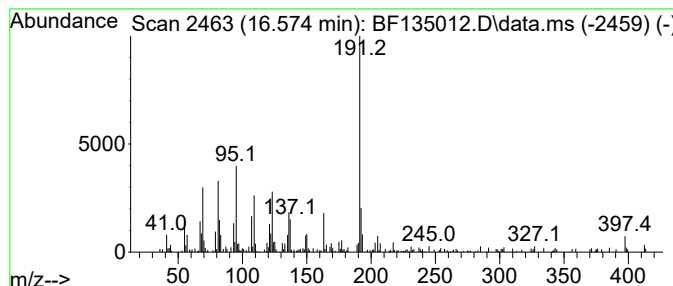
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 17.alpha.H-Trisnorhopane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.574	4.26 ng	179234	Perylene-d12	15.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			17.alpha.H-Trisnorhopane	370	C27H46	053584-59-1	87
2			(7S,7aR,13aS)-9-Methoxy-4,4,7,7a...	344	C22H32O3	1000482-45-3	53
3			17.alpha.(H),21.beta.(H)-Hopane	412	C30H52	013849-96-2	46
4			28-Nor-17.alpha.(H)-hopane	398	C29H50	053584-60-4	46
5			Anthracene, 9-butyl-	234	C18H18	001498-69-7	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083023\
Data File : BF135012.D
Acq On : 30 Aug 2023 19:07
Operator : CG\JU
Sample : 04152-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSITE-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.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
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2-Pentanone, 4-...	4.987	13.2	ng	634362	1	6.769	963408	20.0
2-Propanol, 1-(...	6.575	5.7	ng	273159	1	6.769	963408	20.0
Dipropylene gly...	6.604	3.1	ng	148099	1	6.769	963408	20.0
unknown6.704	6.704	23.1	ng	1115100	1	6.769	963408	20.0
n-Hexadecanoic ...	11.839	16.3	ng	872954	4	11.298	1070770	20.0
Octadecanoic acid	12.633	14.6	ng	586334	5	13.957	805172	20.0
Henicos-1-ene	13.816	3.3	ng	132221	5	13.957	805172	20.0
17.alpha.H-Tris...	16.574	4.3	ng	179234	6	15.427	841670	20.0