

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083023\
 Data File : BF135022.D
 Acq On : 31 Aug 2023 00:49
 Operator : CG\JU
 Sample : 04196-15
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 OR-345-COMP-03

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: BF135022.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.128	4	7	16	rVV2	33501	54112	2.18%	0.303%
2	2.228	20	24	29	rVB	31473	41586	1.67%	0.233%
3	4.998	491	495	502	rVB	92003	105911	4.26%	0.593%
4	5.398	558	563	566	rBV	2596176	2373793	95.41%	13.291%
5	6.410	730	735	738	rBV	2464571	2337381	93.95%	13.087%
6	6.598	764	767	774	rBV	118957	114965	4.62%	0.644%
7	6.769	792	796	800	rBV	926098	745282	29.96%	4.173%
8	7.334	887	892	895	rBV	1749979	1490233	59.90%	8.344%
9	8.051	1009	1014	1017	rBV	1145719	973756	39.14%	5.452%
10	9.128	1193	1197	1200	rBV	2843963	2487884	100.00%	13.930%
11	9.245	1213	1217	1221	rBV	122066	109524	4.40%	0.613%
12	9.810	1309	1313	1316	rBV	1129031	982898	39.51%	5.503%
13	10.598	1443	1447	1450	rBV	1546207	1269478	51.03%	7.108%
14	11.298	1562	1566	1569	rBV	1001440	798593	32.10%	4.471%
15	11.704	1632	1635	1641	rVB	33670	27523	1.11%	0.154%
16	11.839	1653	1658	1669	rBV	339586	365745	14.70%	2.048%
17	12.416	1750	1756	1758	rVB3	43217	47980	1.93%	0.269%
18	12.516	1770	1773	1776	rBV	27749	29752	1.20%	0.167%
19	12.551	1776	1779	1787	rVB7	17226	31872	1.28%	0.178%
20	12.627	1787	1792	1799	rBV3	109940	136808	5.50%	0.766%
21	12.745	1810	1812	1815	rBV	28139	27892	1.12%	0.156%
22	12.898	1834	1838	1841	rBV	1865003	1528471	61.44%	8.558%
23	13.139	1874	1879	1883	rVB6	18273	29018	1.17%	0.162%
24	13.810	1990	1993	2000	rBV2	190680	230574	9.27%	1.291%
25	13.957	2014	2018	2021	rBV	627604	587511	23.61%	3.289%
26	14.451	2099	2102	2113	rVB3	96604	157704	6.34%	0.883%
27	14.821	2162	2165	2171	rVB	59015	67226	2.70%	0.376%
28	15.092	2208	2211	2214	rBV	39682	42793	1.72%	0.240%
29	15.427	2263	2268	2274	rVB	465671	598183	24.04%	3.349%
30	15.915	2348	2351	2355	rBV2	45653	66071	2.66%	0.370%

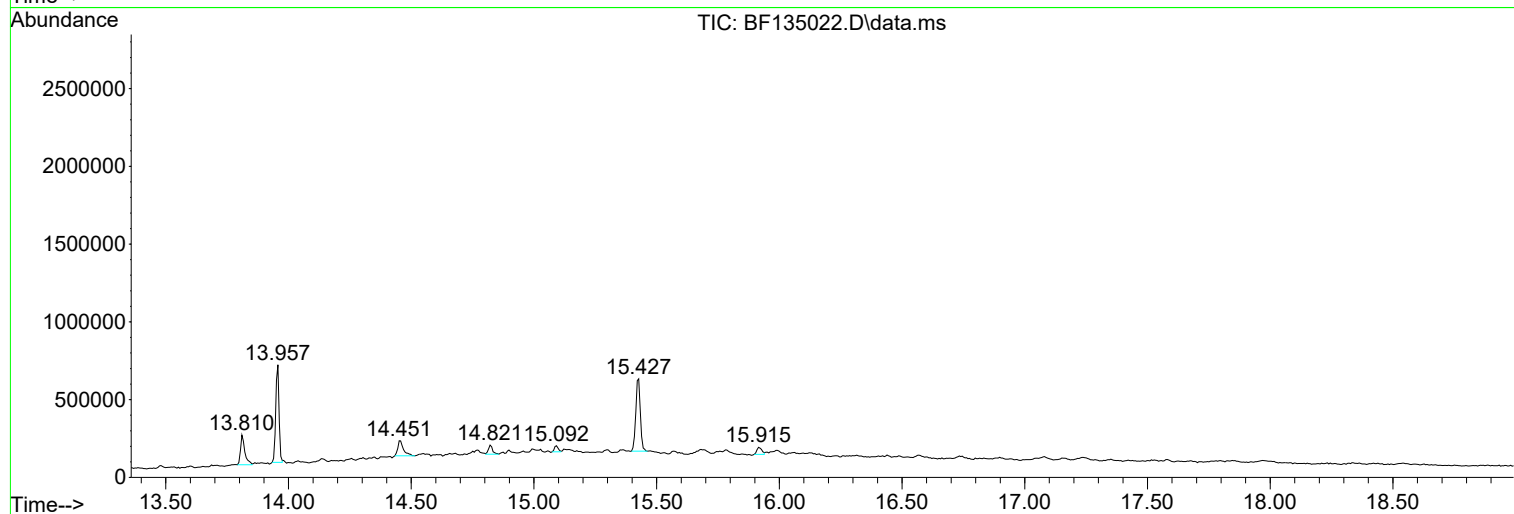
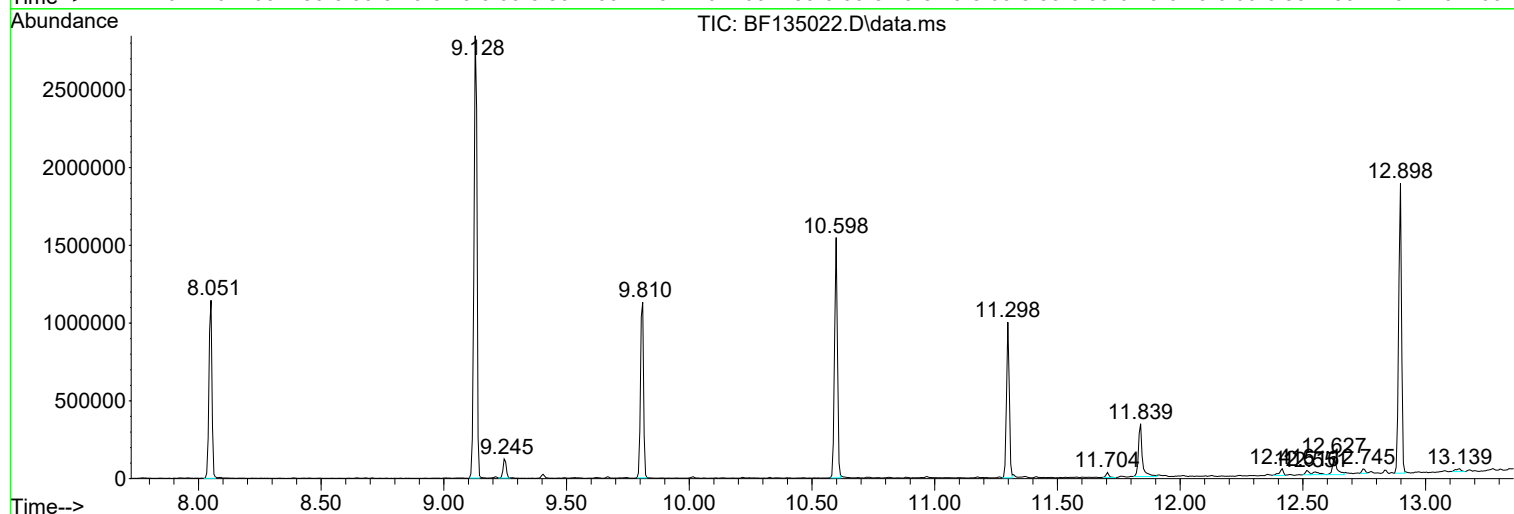
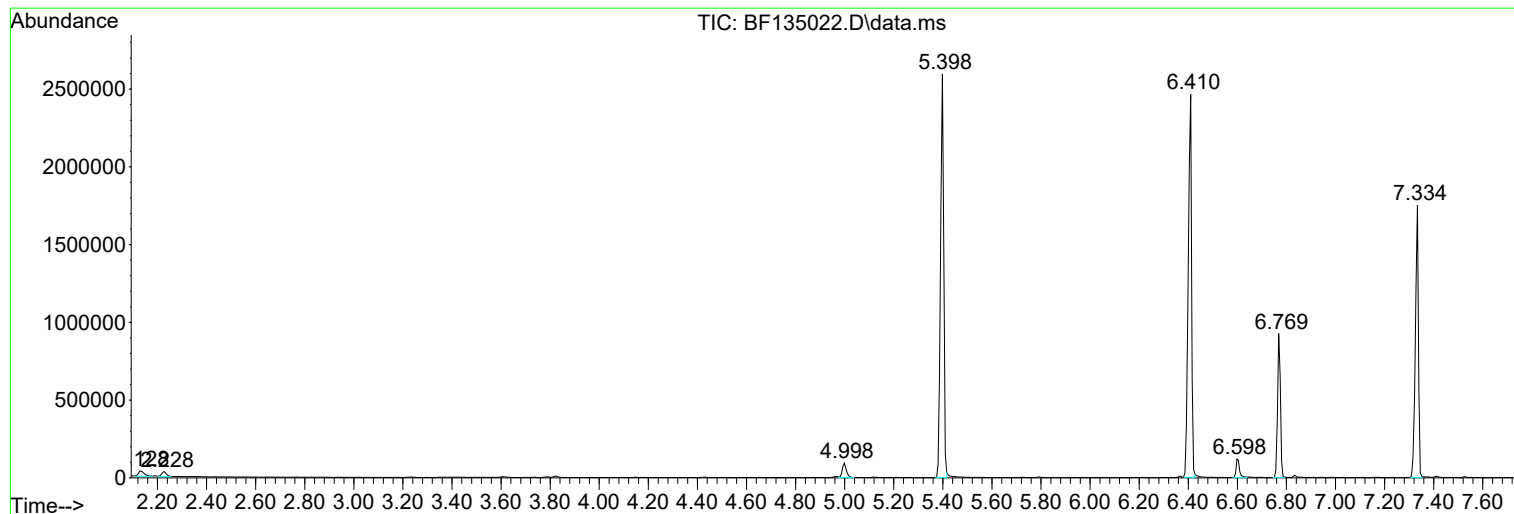
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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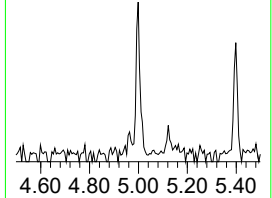
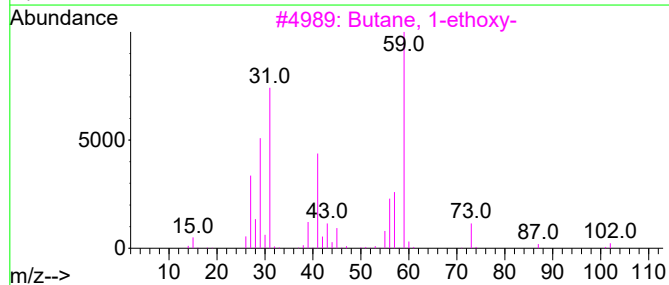
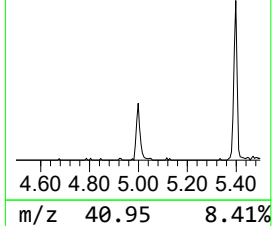
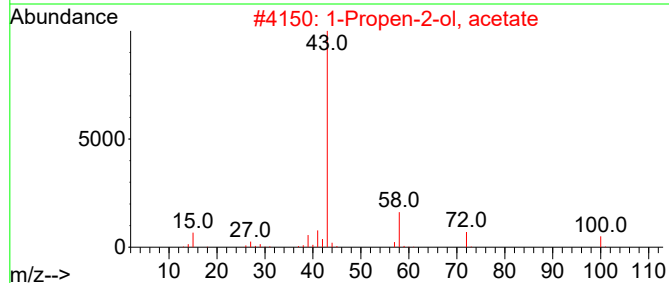
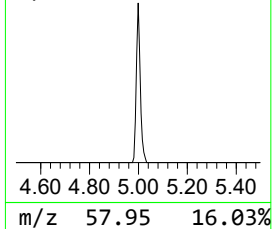
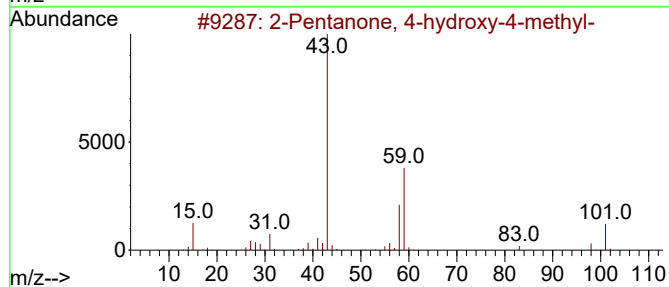
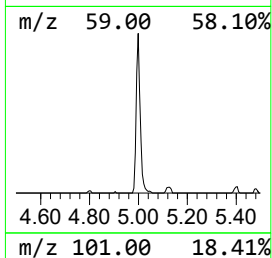
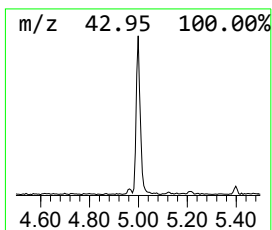
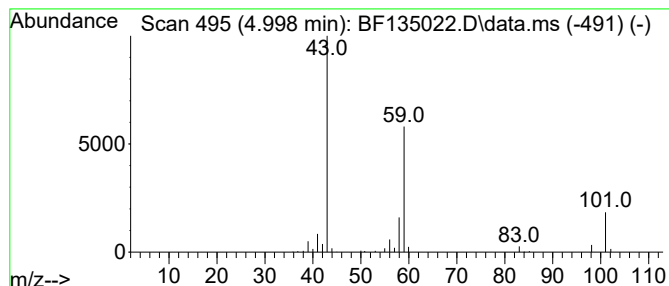
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.998	2.84 ng	105911	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	50		
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9		



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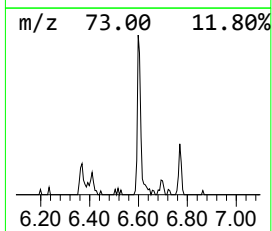
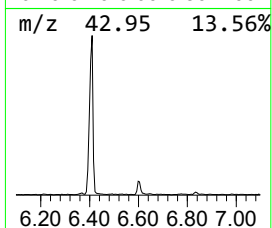
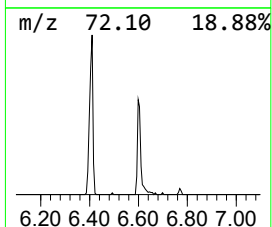
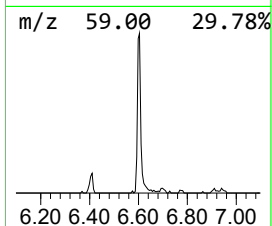
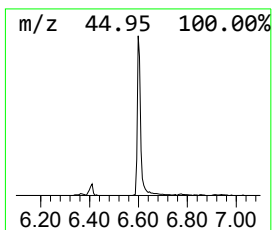
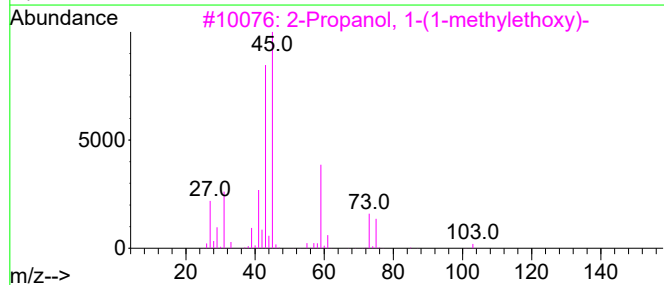
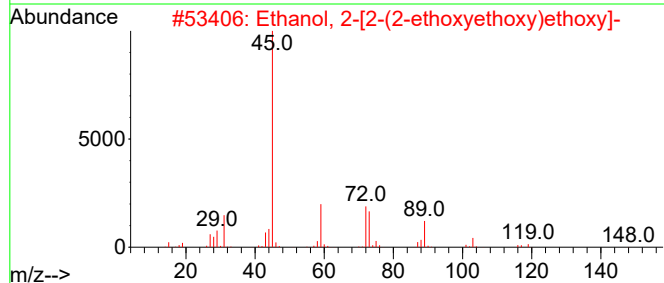
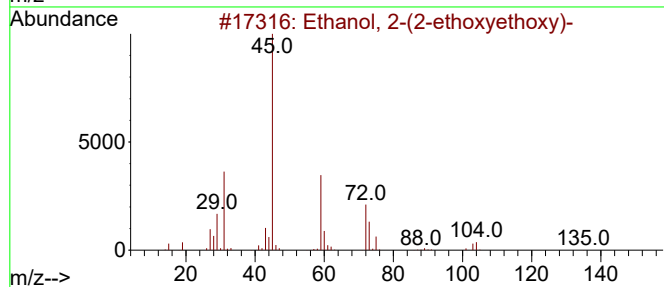
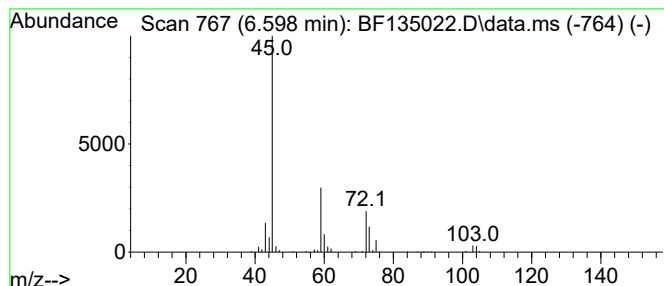
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.598	3.09 ng	114965	1,4-Dichlorobenzene-d4	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	90
2			Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	50
3			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	50
4			Ethane, 1,2-diethoxy-	118	C6H14O2	000629-14-1	38
5			Ethanol, 2-[2-(2-propenyloxy)eth...	146	C7H14O3	015075-50-0	38



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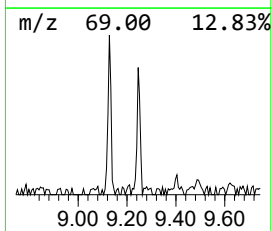
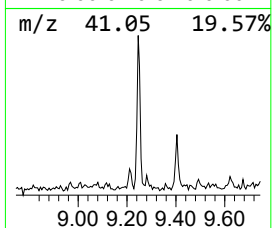
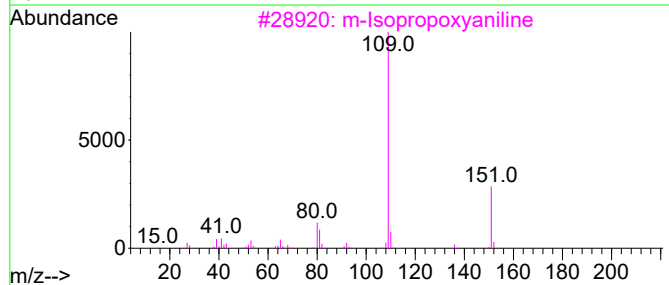
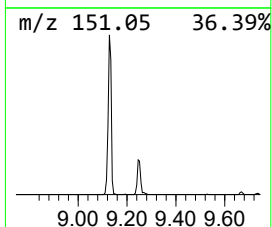
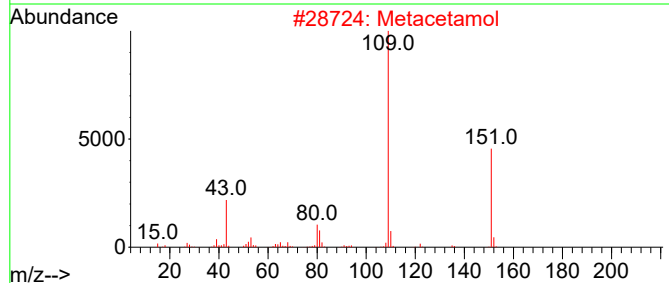
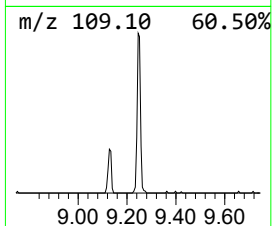
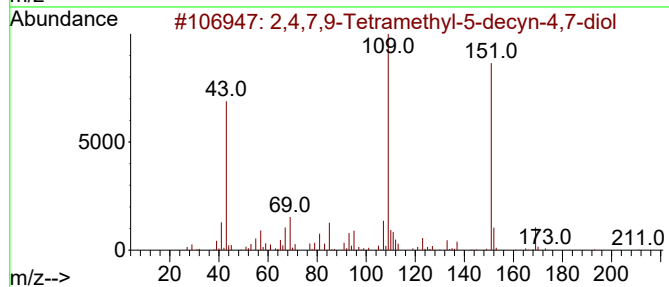
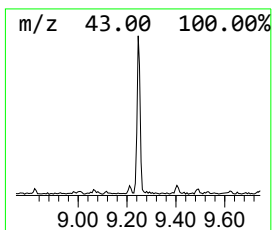
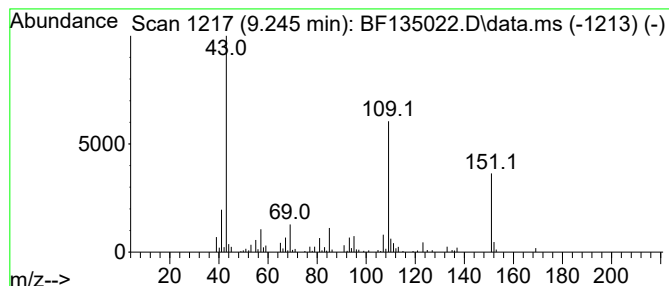
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD			R.T.
9.245	2.23 ng	109524	Acenaphthene-d10			9.810

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2		000126-86-3	74
2	Metacetamol	151	C8H9NO2		000621-42-1	47
3	m-Isopropoxyaniline	151	C9H13NO		041406-00-2	47
4	(-)-10-Camphorsulfonyl chloride	250	C10H15ClO3S		039262-22-1	45
5	4-Amino-2-methylpyrimidine	109	C5H7N3		000074-69-1	43



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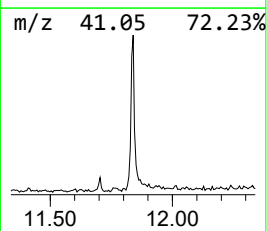
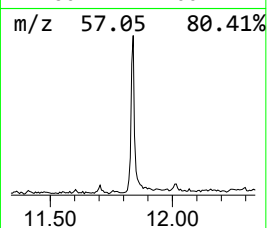
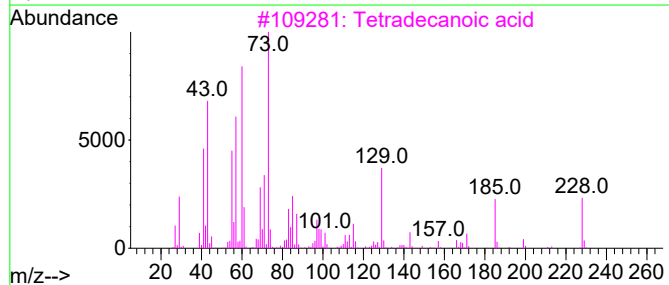
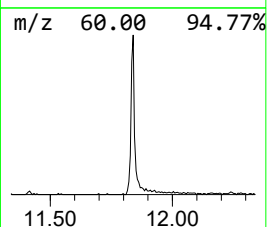
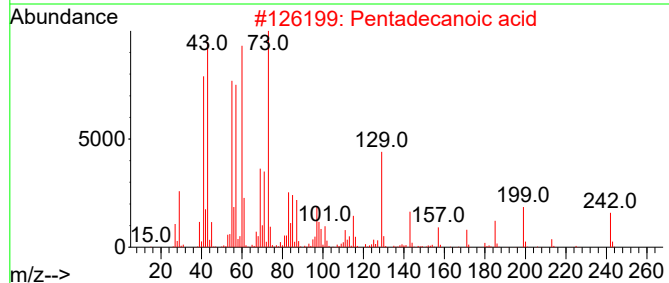
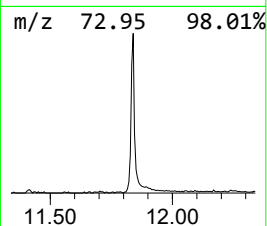
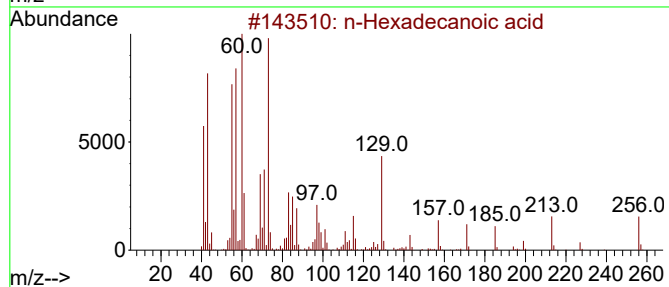
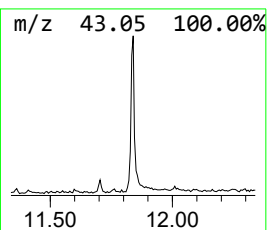
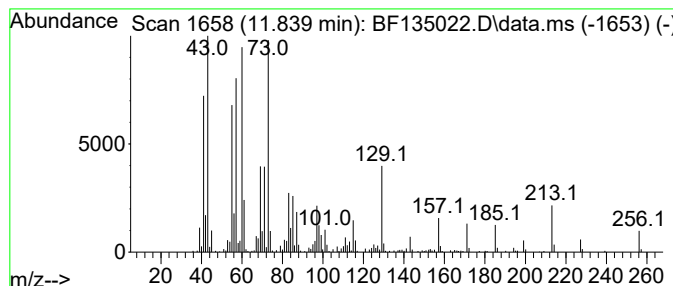
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	9.16 ng	365745	Phenanthrene-d10	11.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4			n-Decanoic acid	172	C10H20O2	000334-48-5	70
5			Tridecanoic acid	214	C13H26O2	000638-53-9	70



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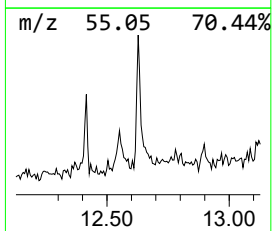
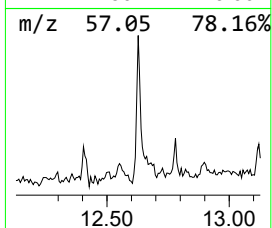
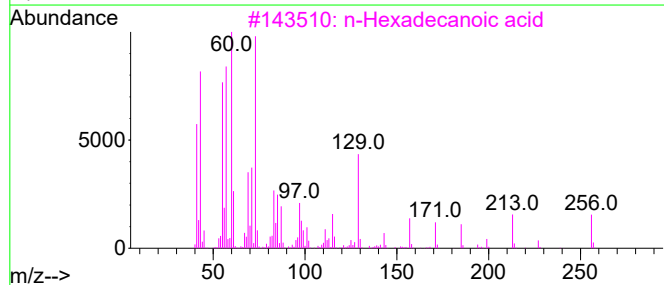
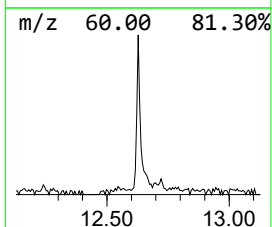
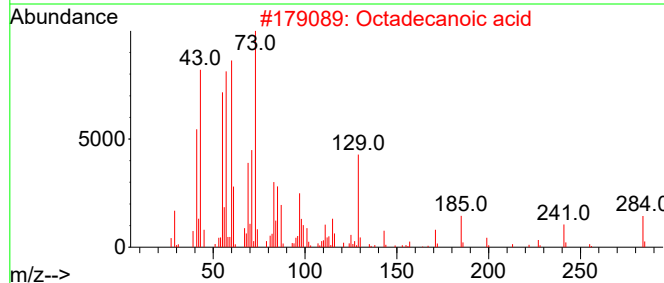
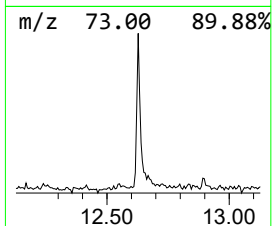
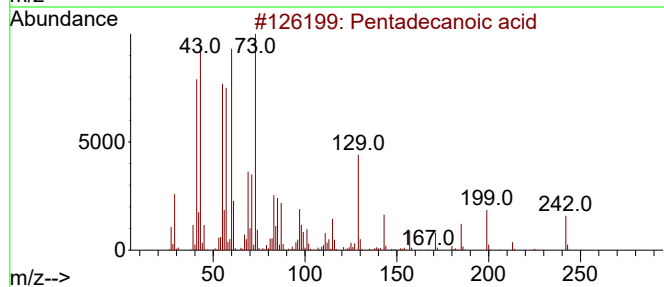
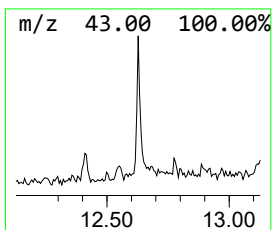
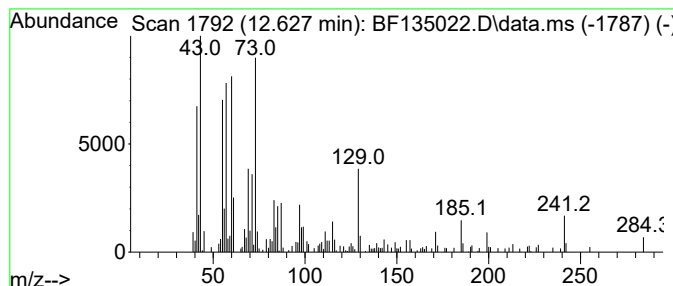
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Peak Number 5 Pentadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.627	3.43 ng	136808	Phenanthrene-d10	11.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
2			Octadecanoic acid	284	C18H36O2	000057-11-4	90
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			n-Decanoic acid	172	C10H20O2	000334-48-5	64



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OR-345-COMP-03

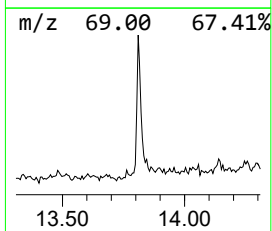
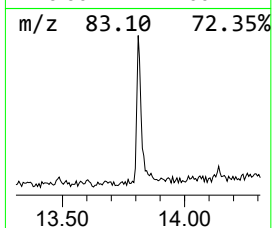
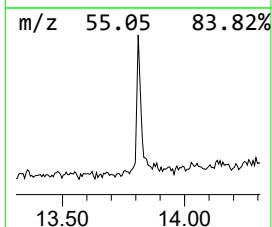
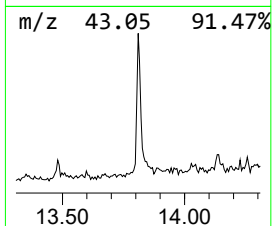
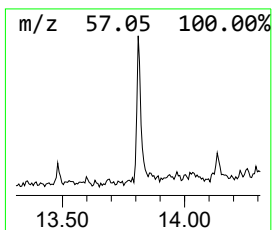
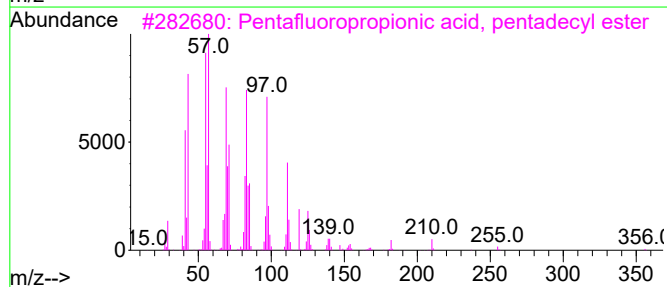
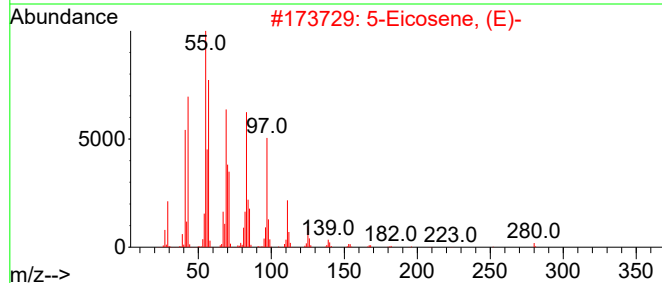
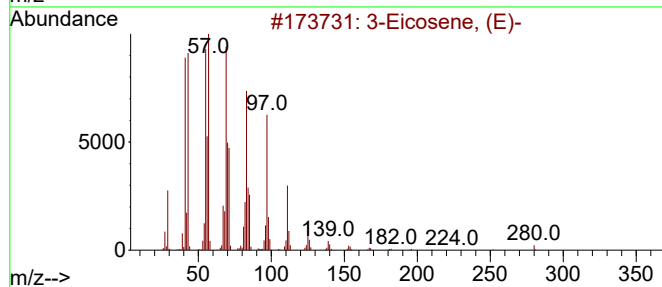
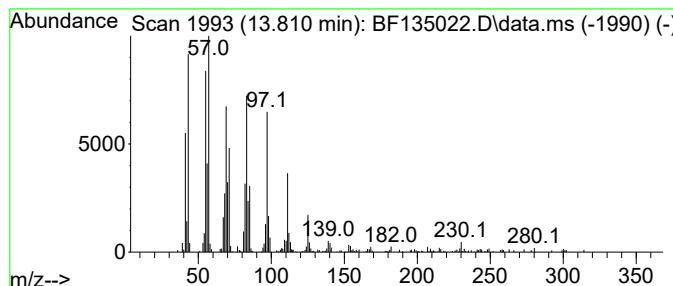
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 3-Eicosene, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.810	7.85 ng	230574	Chrysene-d12	13.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Eicosene, (E)-	280	C20H40	074685-33-9	96
2			5-Eicosene, (E)-	280	C20H40	074685-30-6	95
3			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
4			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
5			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083023\
Data File : BF135022.D
Acq On : 31 Aug 2023 00:49
Operator : CG\JU
Sample : 04196-15
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-345-COMP-03

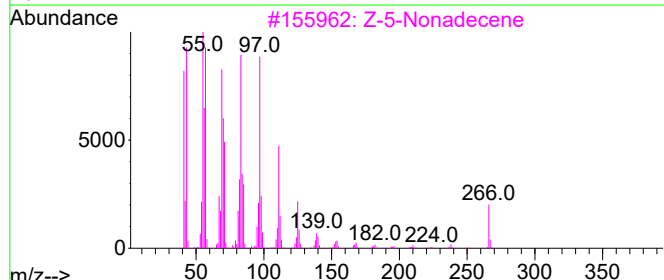
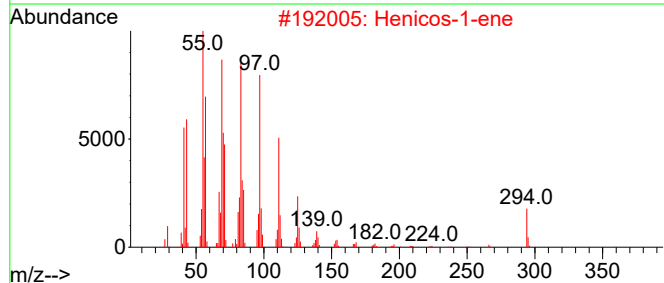
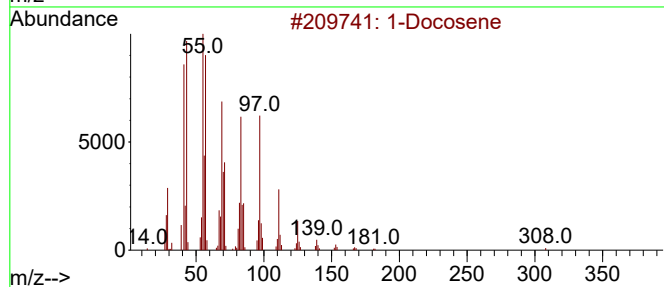
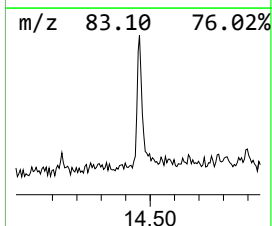
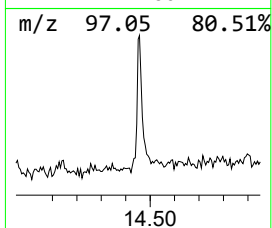
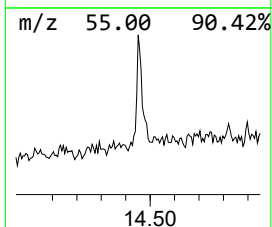
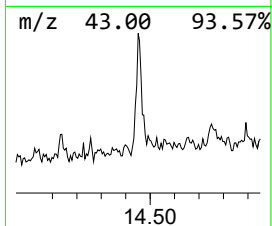
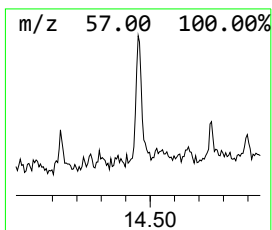
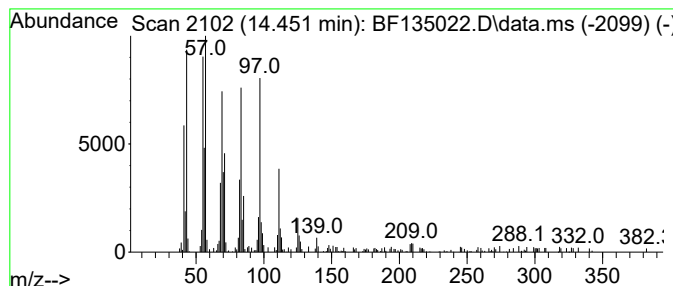
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Docosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.451	5.37 ng	157704	Chrysene-d12	13.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Docosene	308	C22H44	001599-67-3	94
2			Henicos-1-ene	294	C21H42	001599-68-4	94
3			Z-5-Nonadecene	266	C19H38	1000131-11-8	91
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5			1-Octadecanol	270	C18H38O	000112-92-5	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083023\
Data File : BF135022.D
Acq On : 31 Aug 2023 00:49
Operator : CG\JU
Sample : 04196-15
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-345-COMP-03

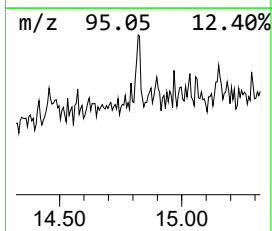
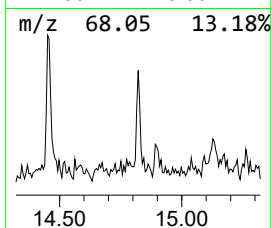
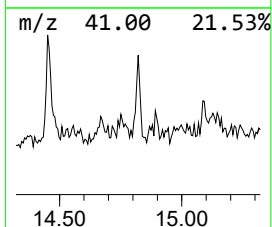
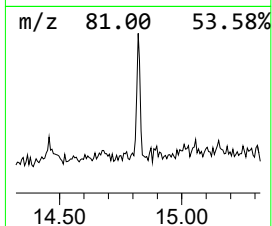
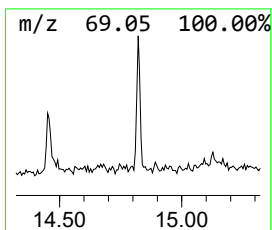
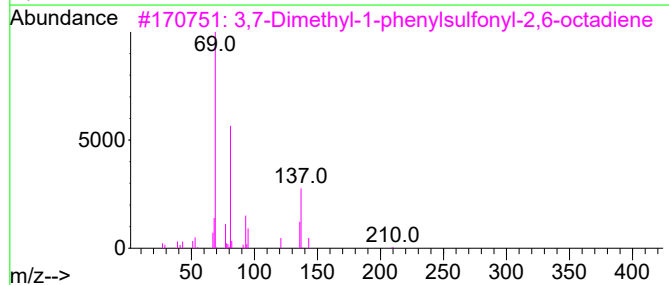
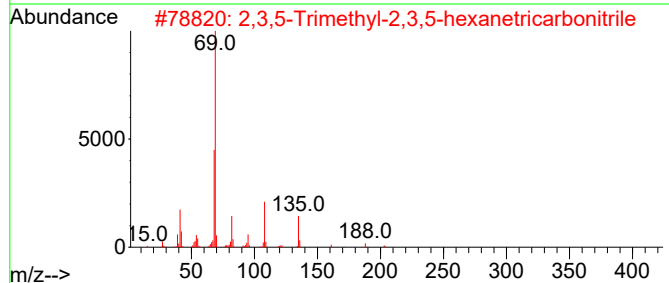
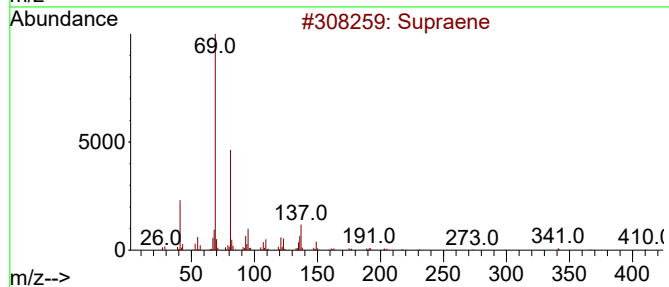
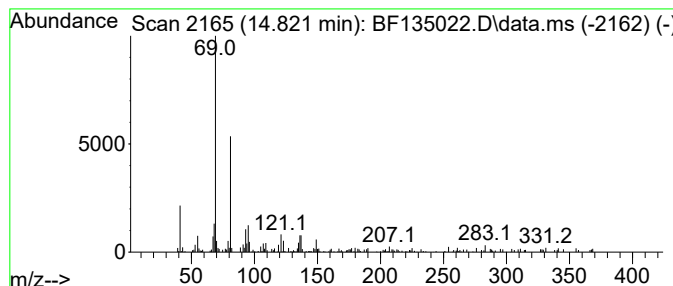
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Supraene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.821	2.25 ng	67226	Perylene-d12	15.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	74
2			2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	64
3			3,7-Dimethyl-1-phenylsulfonyl-2,...	278	C16H22O2S	1000432-27-5	59
4			2-propenoic acid, 2-methyl-, 4-[...]	283	C13H17NO4S	1000401-94-0	59
5			Furan, 3-(4-methyl-3-pentenyl)-	150	C10H14O	000539-52-6	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083023\
Data File : BF135022.D
Acq On : 31 Aug 2023 00:49
Operator : CG\JU
Sample : 04196-15
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
OR-345-COMP-03

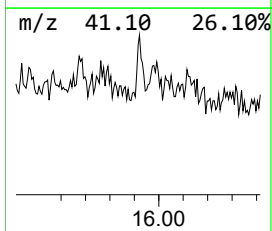
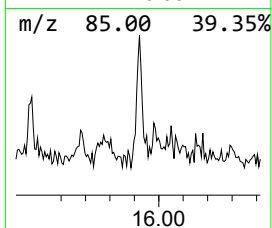
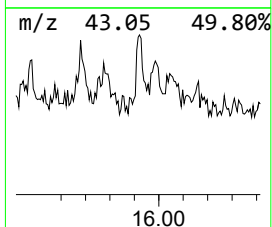
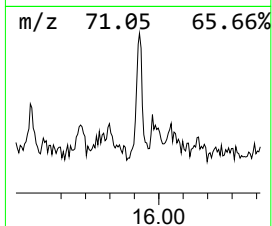
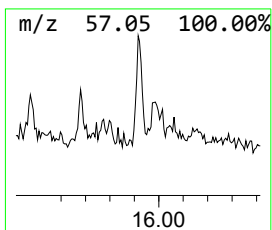
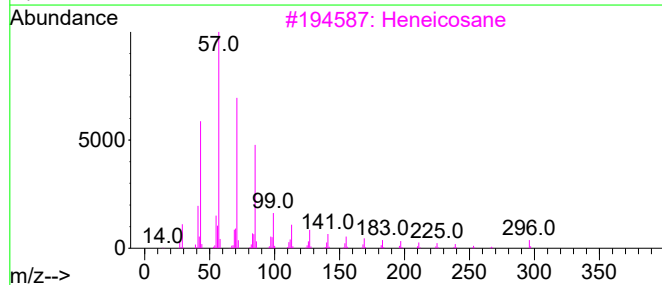
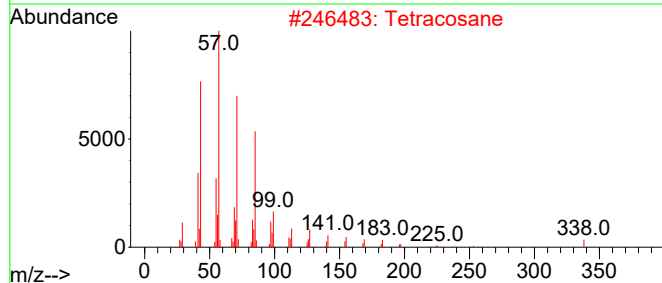
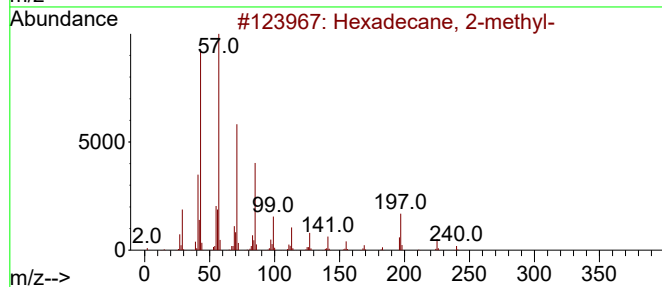
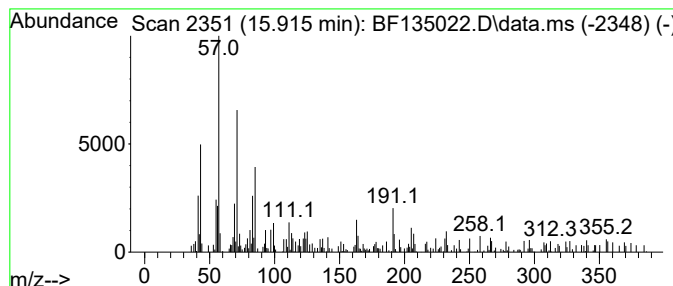
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexadecane, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.915	2.21 ng	66071	Perylene-d12	15.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane, 2-methyl-	240	C17H36	001560-92-5	55
2			Tetracosane	338	C24H50	000646-31-1	55
3			Heneicosane	296	C21H44	000629-94-7	55
4			1-Bromoeicosane	360	C20H41Br	004276-49-7	53
5			Tricosane	324	C23H48	000638-67-5	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083023\
Data File : BF135022.D
Acq On : 31 Aug 2023 00:49
Operator : CG\JU
Sample : 04196-15
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-345-COMP-03

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
2-Pentanone, 4-...	4.998	2.8	ng	105911	1	6.769	745282	20.0
Ethanol, 2-(2-e...	6.598	3.1	ng	114965	1	6.769	745282	20.0
2,4,7,9-Tetrame...	9.245	2.2	ng	109524	3	9.810	982898	20.0
n-Hexadecanoic ...	11.839	9.2	ng	365745	4	11.298	798593	20.0
Pentadecanoic acid	12.627	3.4	ng	136808	4	11.298	798593	20.0
3-Eicosene, (E)-	13.810	7.8	ng	230574	5	13.957	587511	20.0
1-Docosene	14.451	5.4	ng	157704	5	13.957	587511	20.0
Supraene	14.821	2.3	ng	67226	6	15.427	598183	20.0
Hexadecane, 2-m...	15.915	2.2	ng	66071	6	15.427	598183	20.0