LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041923\
Data File : BF132922.D
Acq On : 19 Apr 2023 20:40
Operator : CG\JU
Sample : 02366-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20230330-COMP-8

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-BF041723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132922.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.116	173	175	190	rBV	78690	180824	1.66%	0.265%
2	4.963	480	489	501	rVB	2150600	3176859	29.11%	4.659%
3	5.375	553	559	562	rBV	7367629	8433089	77.28%	12.369%
4	5.769	623	626	633	rVB	256215	219256	2.01%	0.322%
5	6.393	726	732	735	rBV	7218854	8774612	80.41%	12.869%
6	6.763	791	795	798	rVB	1956035	1530190	14.02%	2.244%
7	7.328	885	891	894	rBV	5960765	5519920	50.59%	8.096%
8	8.045	1009	1013	1016	rBV	2852264	2116861	19.40%	3.105%
9	9.128	1192	1197	1200	rBV	9813281	8997917	82.46%	13.197%
10	9.798	1307	1311	1314	rBV	3276174	2440306	22.36%	3.579%
11	10.516	1429	1433	1436	rVB	400746	357841	3.28%	0.525%
12	10.586	1440	1445	1448	rBV	6923998	6722488	61.61%	9.860%
13	11.281	1559	1563	1566	rBV	3332721	2688644	24.64%	3.943%
14	11.816	1650	1654	1658	rBV	673065	682689	6.26%	1.001%
15	12.598	1785	1787	1795	rBV	103797	129070	1.18%	0.189%
16	12.875	1829	1834	1837	rBV	10814954	10911731	100.00%	16.004%
17	13.769	1983	1986	2001	rBV2	602886	906794	8.31%	1.330%
18	13.916	2007	2011	2014	rBV	2353672	2162789	19.82%	3.172%
19	14.098	2039	2042	2050	rVB	167069	147385	1.35%	0.216%
20	14.404	2090	2094	2100	rBV	178517	170838	1.57%	0.251%
21	14.704	2141	2145	2150	rBV	122095	113198	1.04%	0.166%
22	15.033	2197	2201	2209	rBV	95099	115093	1.05%	0.169%
23	15.345	2248	2254	2260	rBV	1420209	1683370	15.43%	2.469%

Sum of corrected areas: 68181764

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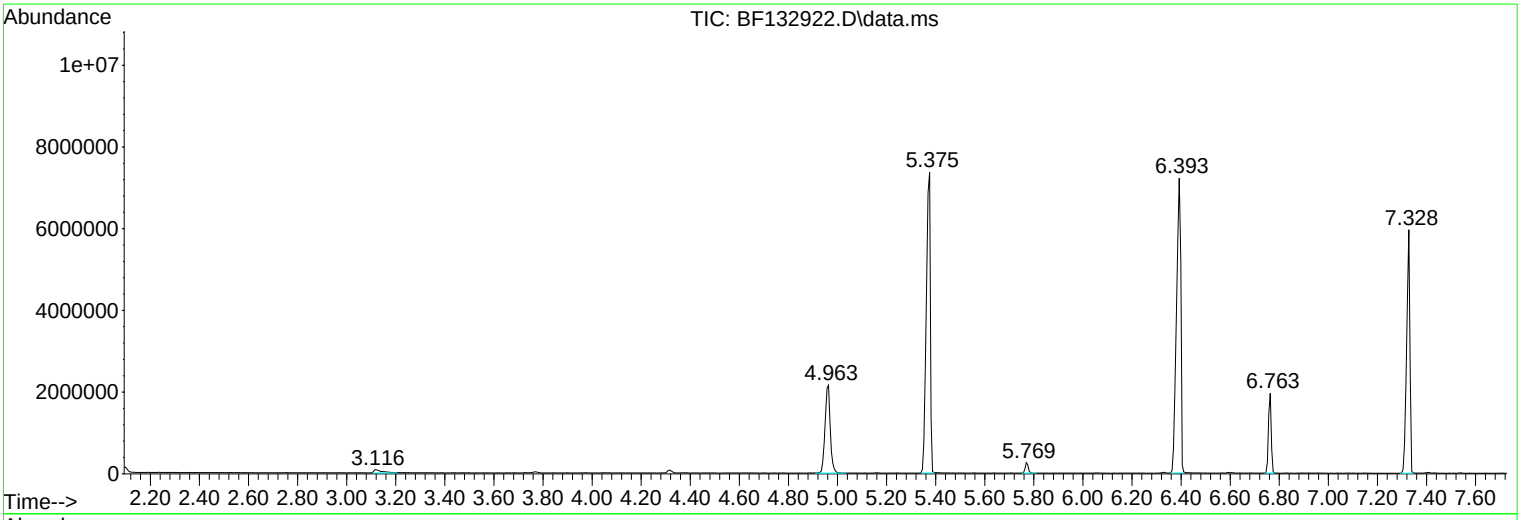
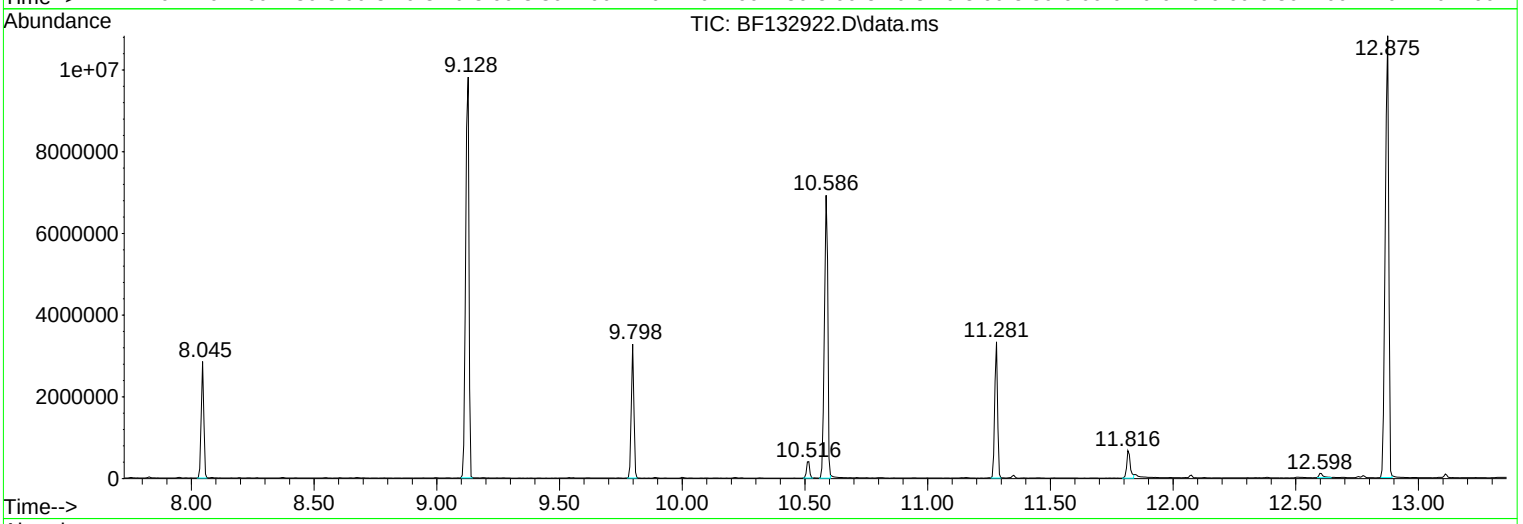
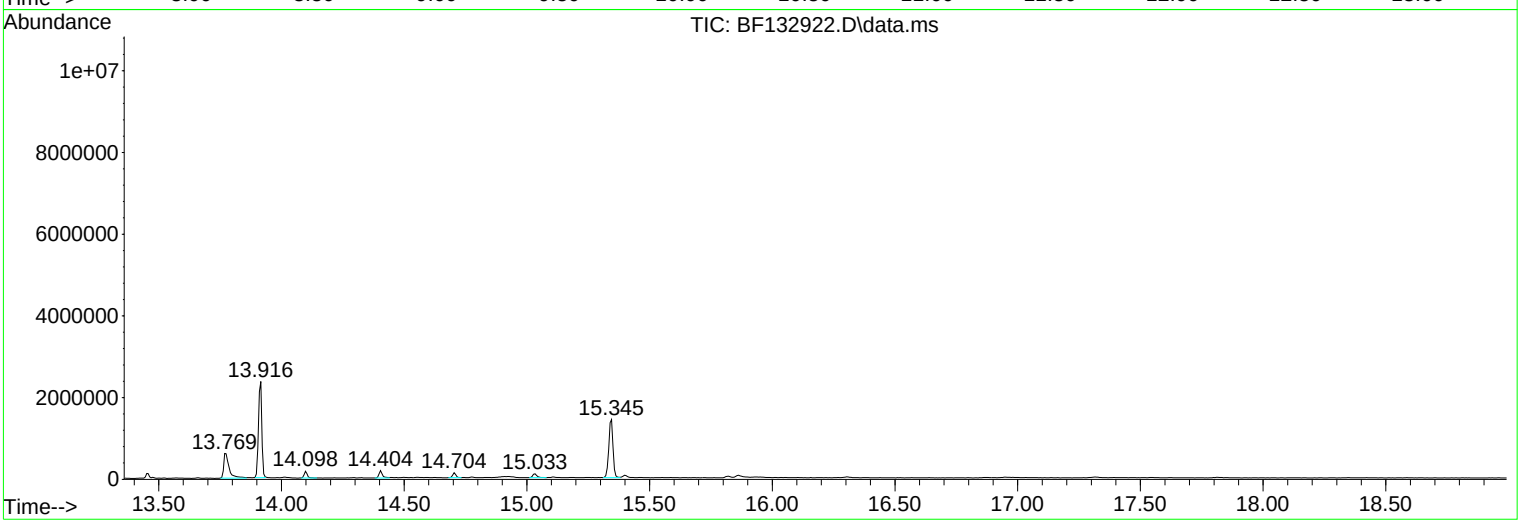
ClientSampleId :
20230330-COMP-8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF041723.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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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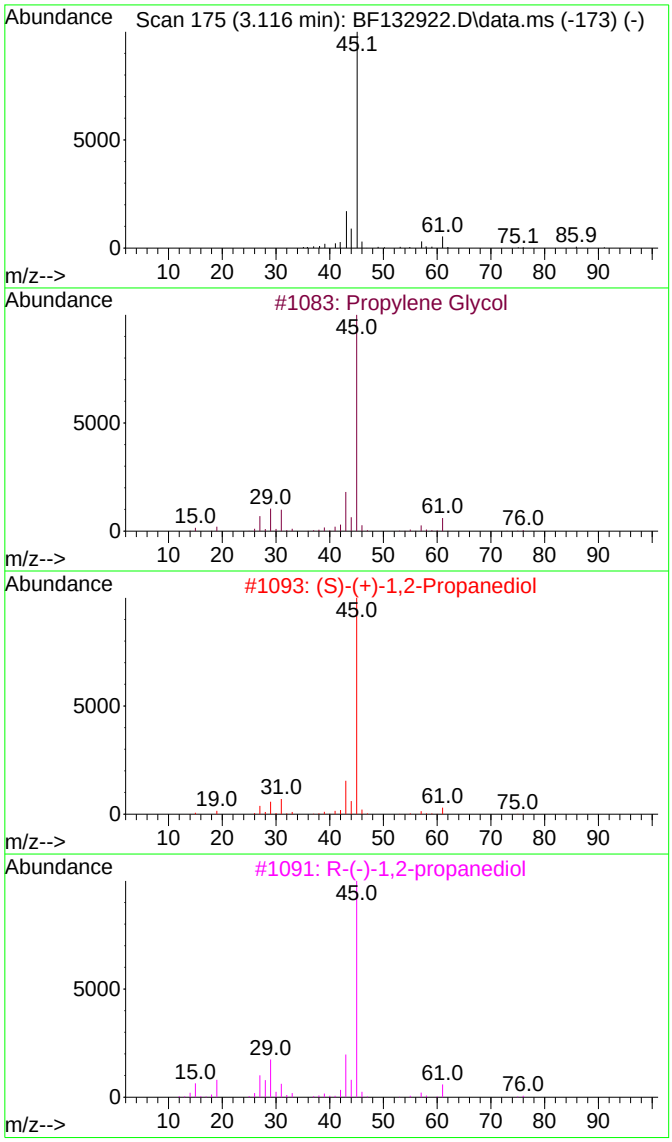
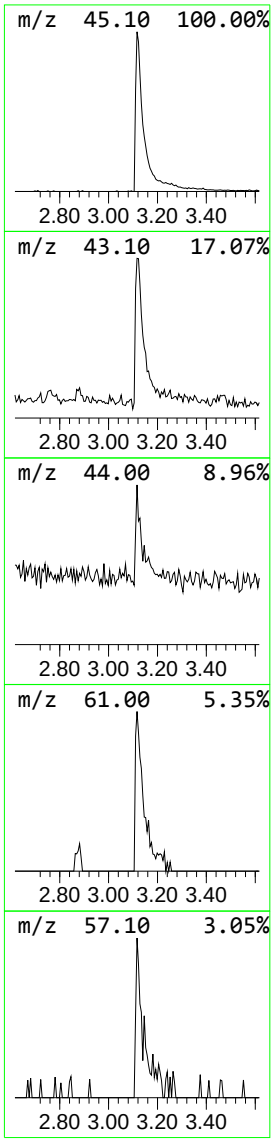
****

Peak Number 1 Propylene Glycol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.116	2.36 ng	180824	1,4-Dichlorobenzene-d4	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	78
2	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	56
3	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
4	2-Hexanol	102	C6H14O	000626-93-7	9
5	Ethanol, 2-methoxy-, carbonate (...	178	C7H14O5	000626-84-6	9





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Instrument :
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ClientSampleId :
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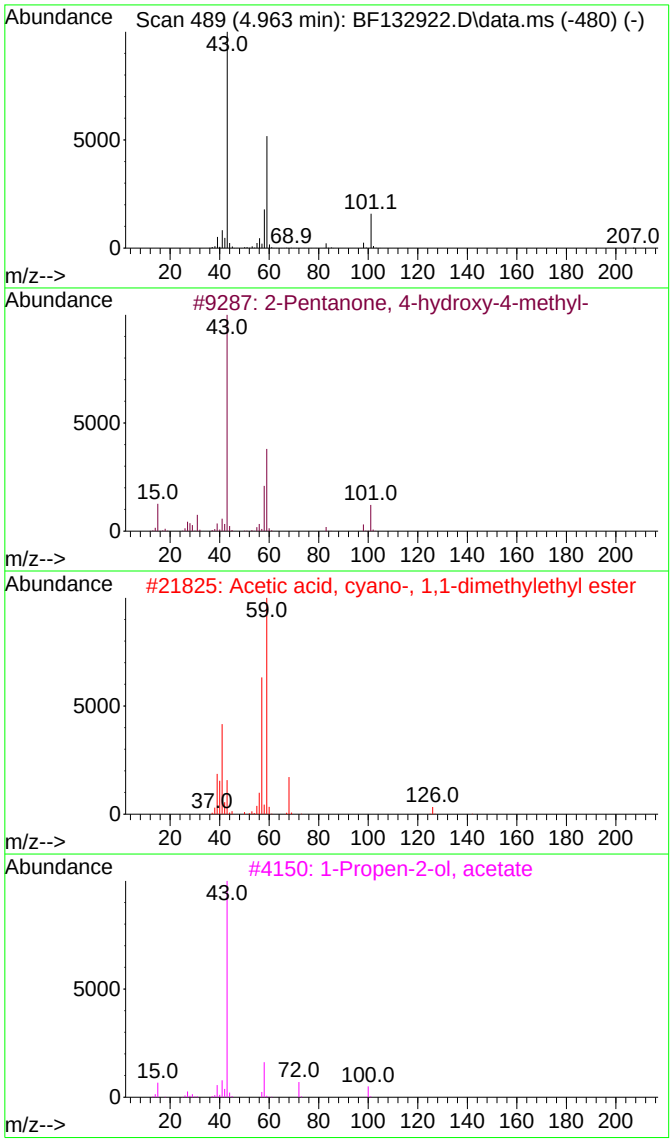
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF041723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

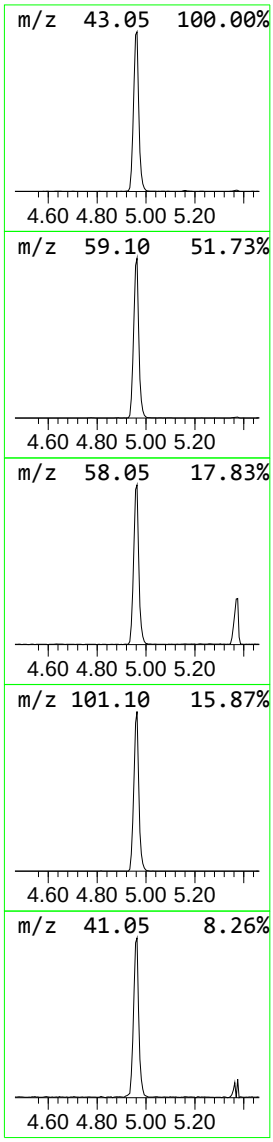
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.963	41.52 ng	3176860	1,4-Dichlorobenzene-d4	6.763

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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9





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Instrument :
BNA_F
ClientSampleId :
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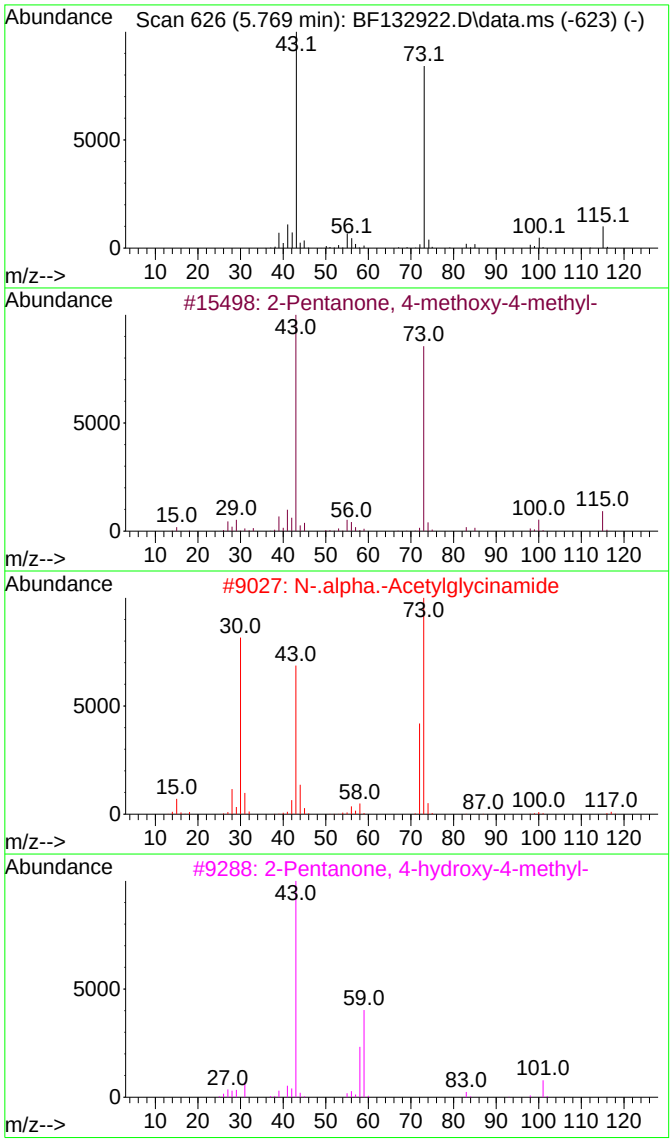
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF041723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

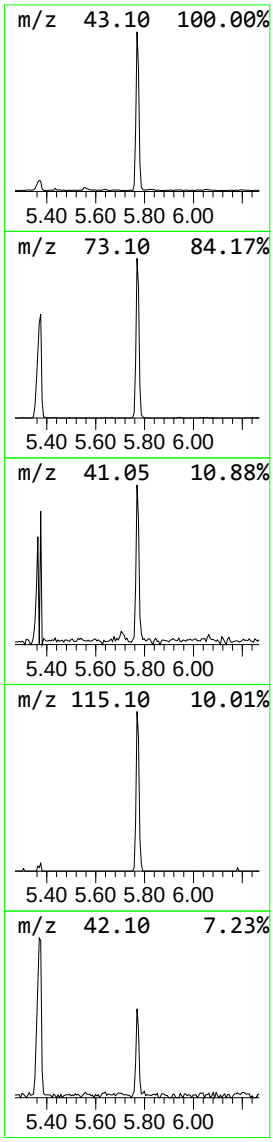
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.769	2.87 ng	219256	1,4-Dichlorobenzene-d4	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	38
3	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	10
4	2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9





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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF041723.M
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TIC Library : C:\Database\NIST20.L
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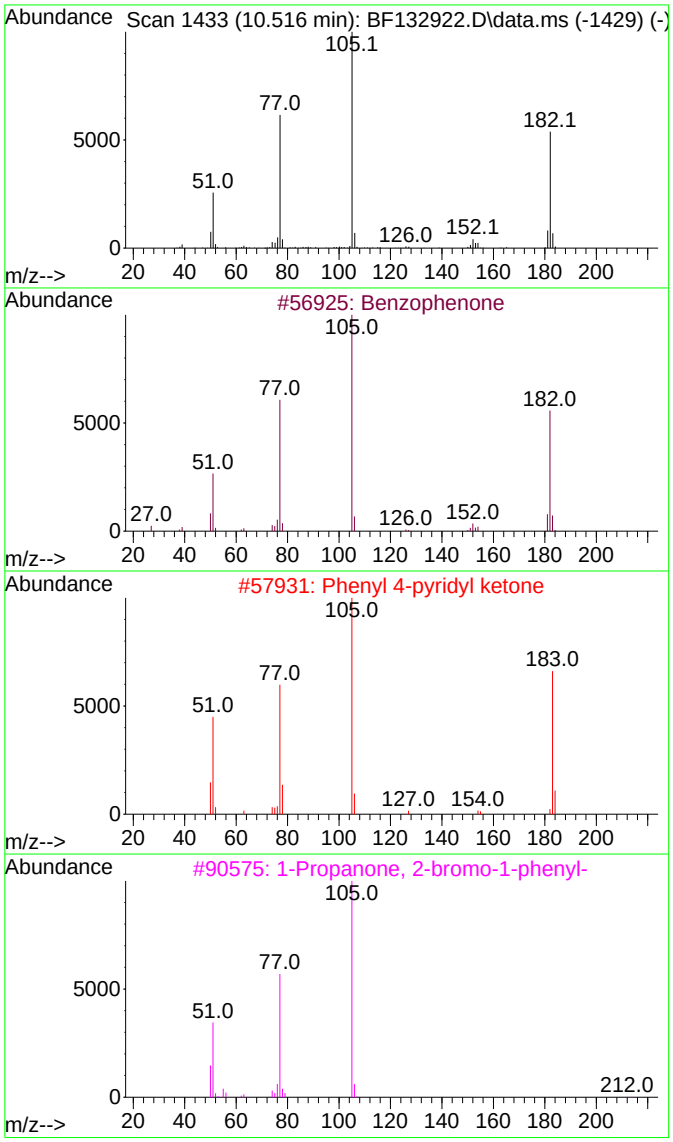
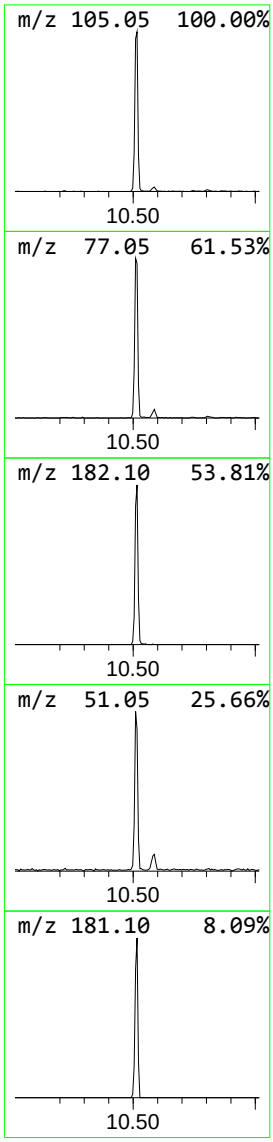
Peak Number 4 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.516	2.93 ng	357841	Acenaphthene-d10	9.798

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	50
3	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
4	Benzoic acid, phenyl ester	198	C13H10O2	000093-99-2	47
5	2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	47





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Sample : 02366-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20230330-COMP-8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF041723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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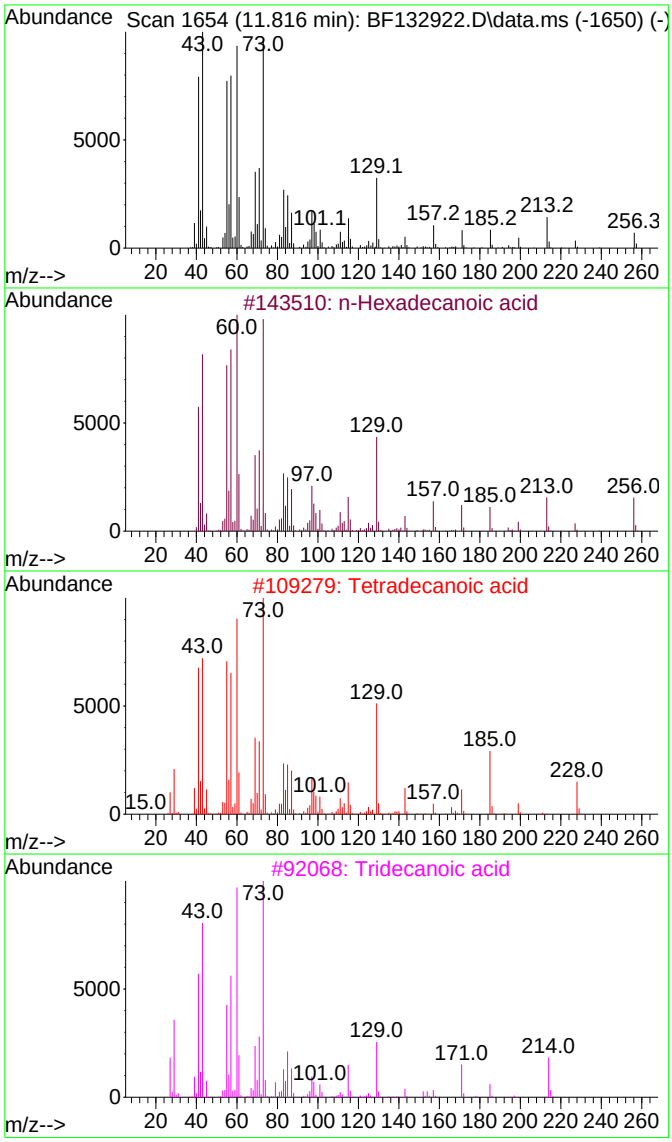
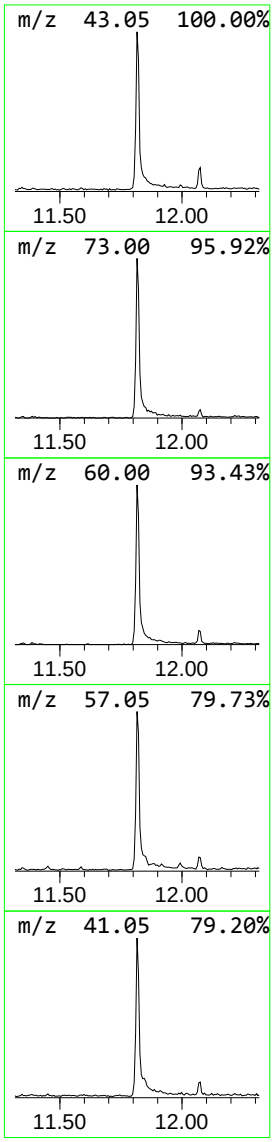
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.816	5.08 ng	682689	Phenanthrene-d10	11.281

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	90
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5	Undecanoic acid	186	C11H22O2	000112-37-8	87





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TIC Library : C:\Database\NIST20.L
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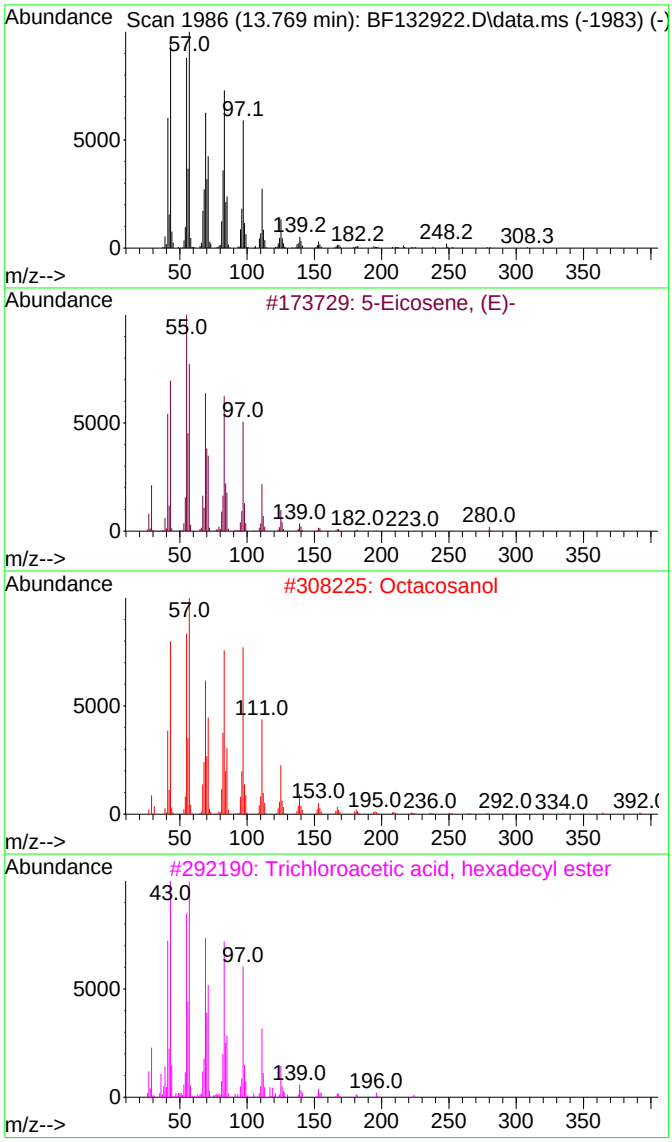
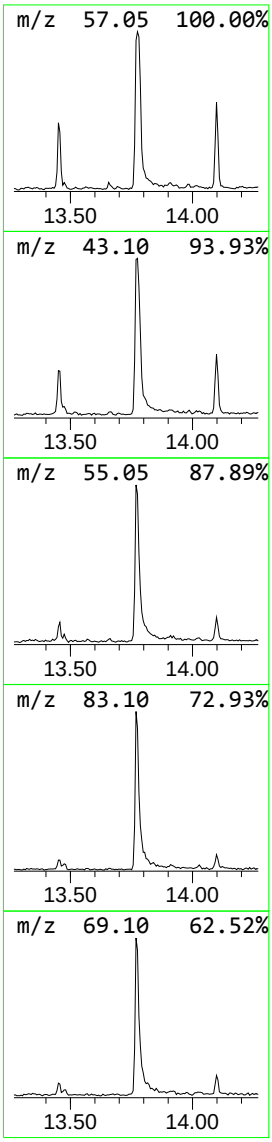
Peak Number 6 5-Eicosene, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.769	8.39 ng	906794	Chrysene-d12	13.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	97
2	Octacosanol	410	C28H58O	000557-61-9	94
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91





Tentatively Identified Compound (LSC) summary

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propylene Glycol	3.116	2.4	ng	180824	1	6.763	1530190	20.0
2-Pentanone, 4-...	4.963	41.5	ng	3176860	1	6.763	1530190	20.0
2-Pentanone, 4-...	5.769	2.9	ng	219256	1	6.763	1530190	20.0
Benzophenone	10.516	2.9	ng	357841	3	9.798	2440310	20.0
n-Hexadecanoic ...	11.816	5.1	ng	682689	4	11.281	2688640	20.0
5-Eicosene, (E)-	13.769	8.4	ng	906794	5	13.916	2162790	20.0