LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091523\
Data File : BF135282.D
Acq On : 15 Sep 2023 16:43
Operator : CG\JU
Sample : 04409-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-3(0-2)COMP

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-BF091123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135282.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.122	3	6	17	rVB	44083	71097	3.22%	0.450%
2	4.993	490	494	499	rBV	66009	84342	3.82%	0.534%
3	5.393	557	562	565	rBV	2251540	2070008	93.66%	13.094%
4	6.398	729	733	736	rBV	2134271	2065271	93.45%	13.064%
5	6.592	763	766	779	rBV	61444	74447	3.37%	0.471%
6	6.757	790	794	798	rBV	866699	672919	30.45%	4.257%
7	7.322	885	890	893	rBV	1436463	1346868	60.94%	8.520%
8	8.034	1007	1011	1015	rBV	1010489	867806	39.27%	5.490%
9	9.116	1190	1195	1198	rBV	2543054	2210016	100.00%	13.980%
10	9.233	1211	1215	1219	rBV	190382	168987	7.65%	1.069%
11	9.792	1305	1310	1313	rBV	1084106	872363	39.47%	5.518%
12	10.586	1441	1445	1448	rBV	1393983	1230583	55.68%	7.784%
13	11.286	1560	1564	1567	rBV	869018	774703	35.05%	4.901%
14	11.822	1651	1655	1666	rBV	307884	336029	15.20%	2.126%
15	12.398	1750	1753	1756	rVB	31724	26473	1.20%	0.167%
16	12.610	1786	1789	1794	rBV	103026	126399	5.72%	0.800%
17	12.880	1831	1835	1839	rBV	1613725	1497331	67.75%	9.472%
18	13.374	1916	1919	1924	rVB	98511	93175	4.22%	0.589%
19	13.945	2012	2016	2020	rBV	642033	593948	26.88%	3.757%
20	15.415	2262	2266	2271	rVB	508082	625654	28.31%	3.958%

Sum of corrected areas: 15808419

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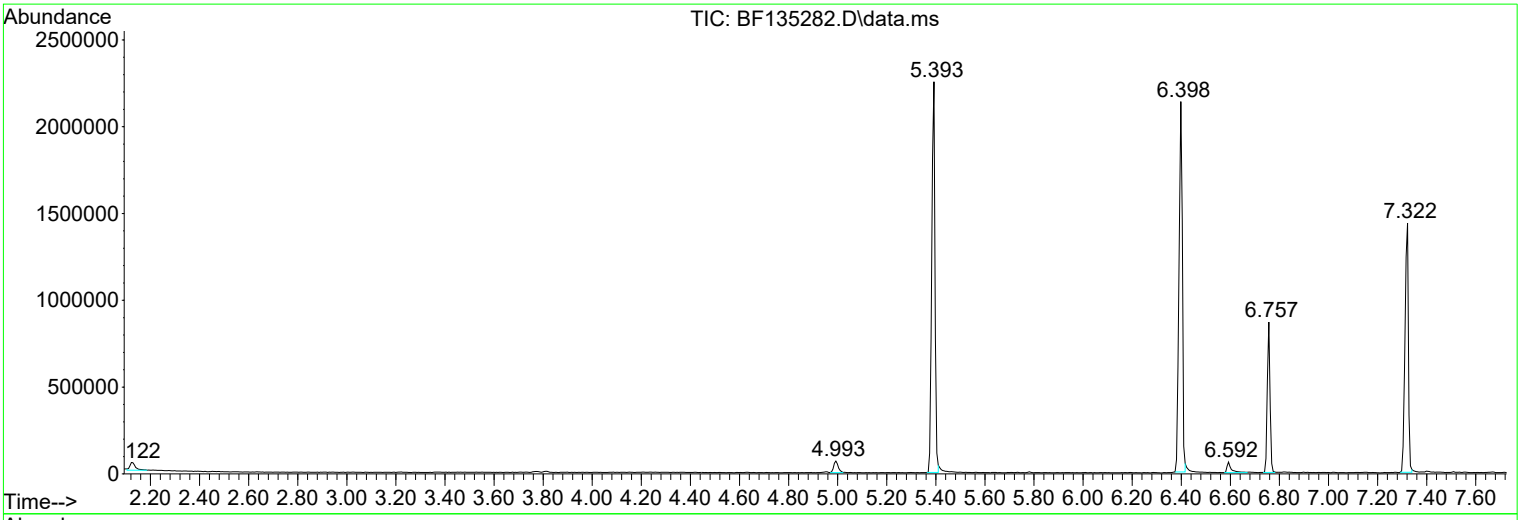
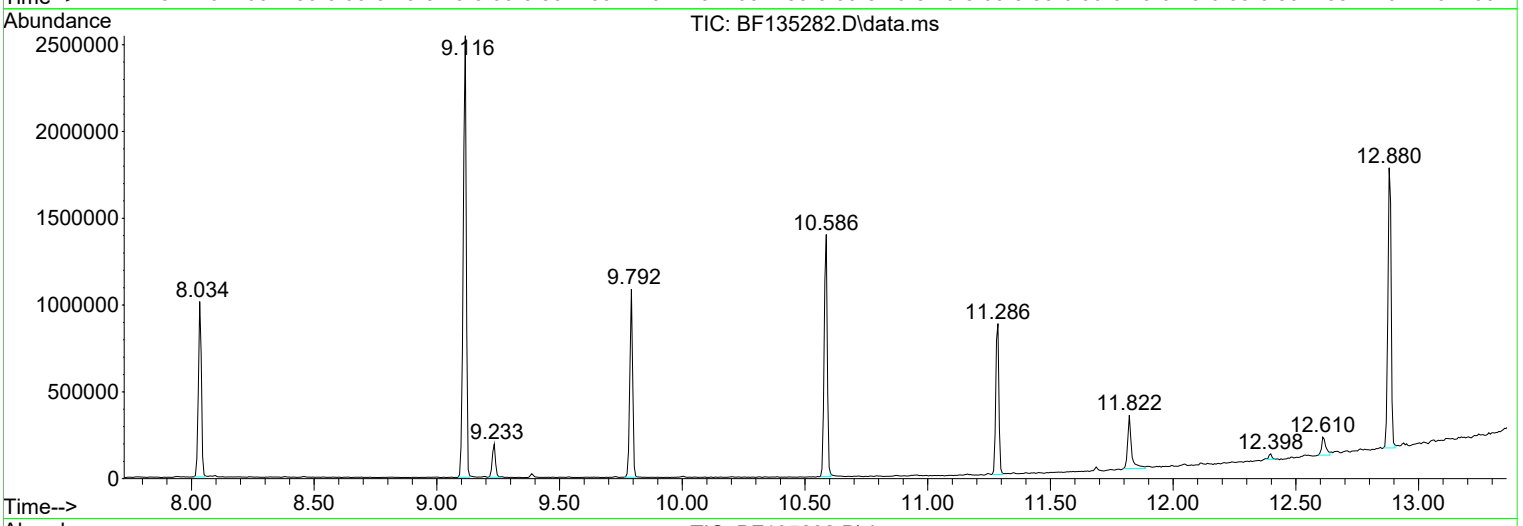
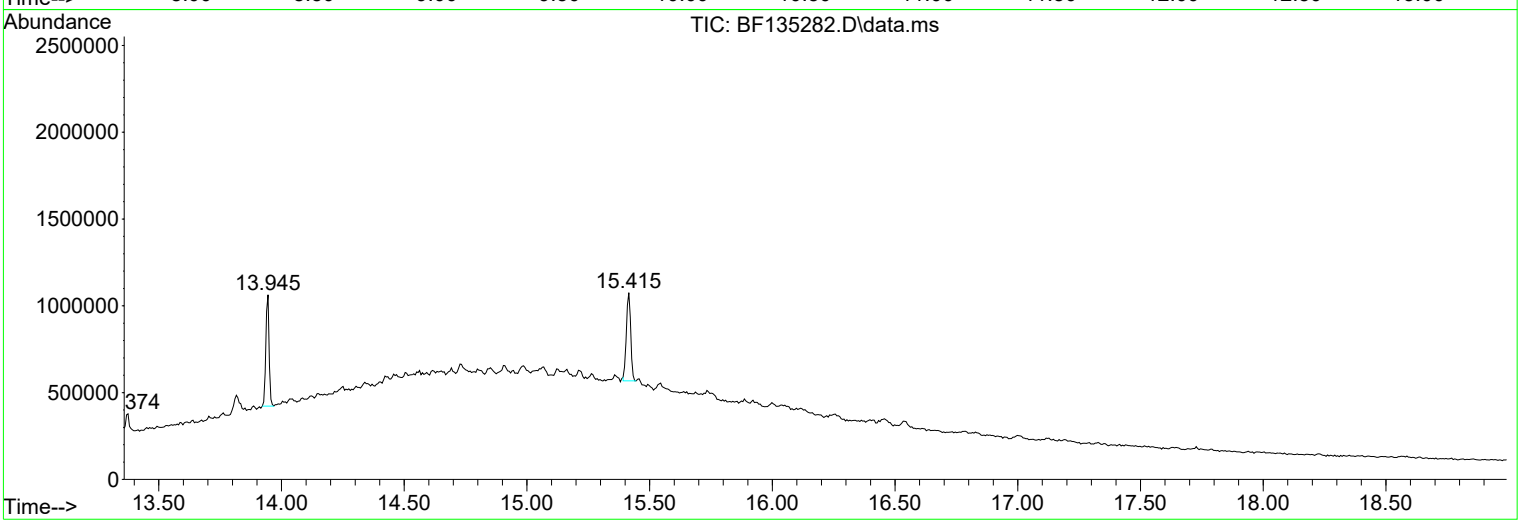
ClientSampleId :
WC-3(0-2)COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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

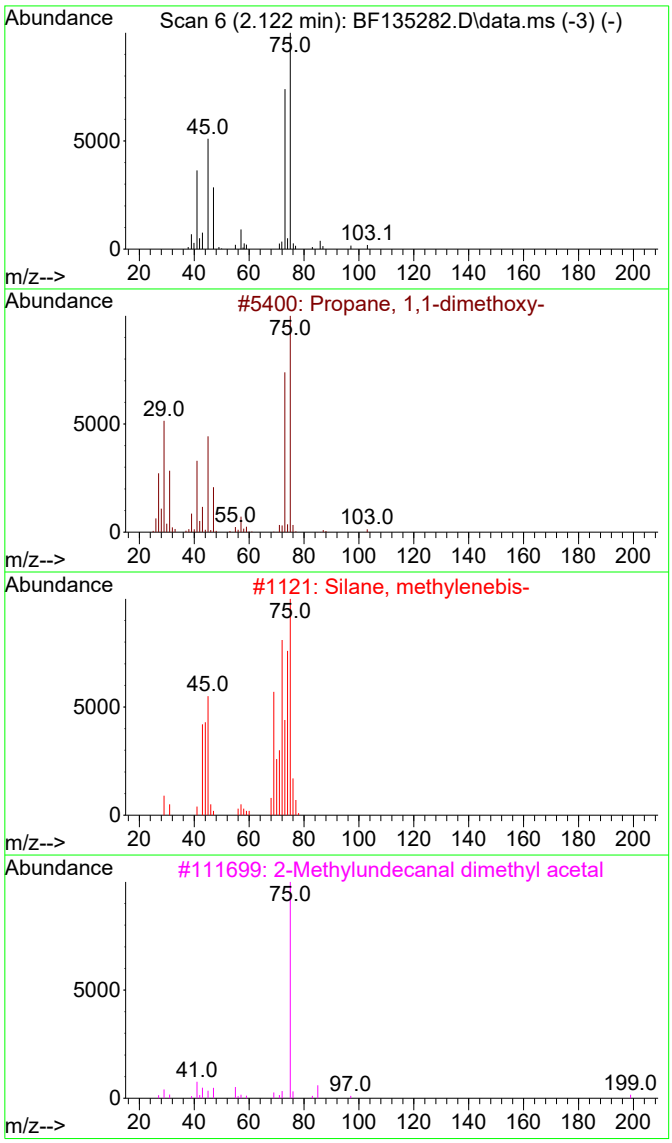
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

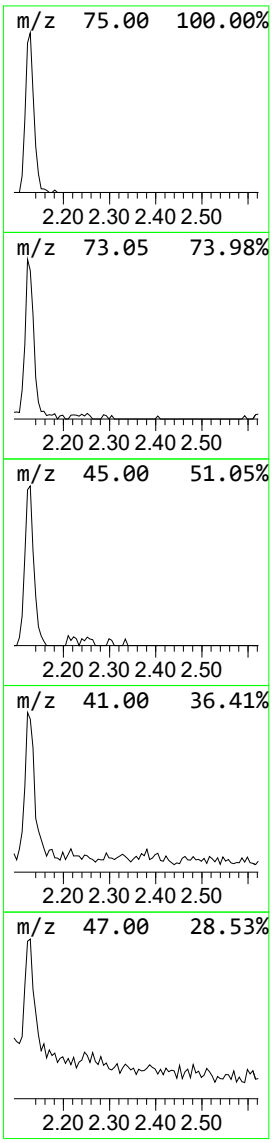
****

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.122	2.11 ng	71097	1,4-Dichlorobenzene-d4	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	78
2	Silane, methylenebis-	76	CH8Si2	001759-88-2	50
3	2-Methylundecanal dimethyl acetal	230	C14H30O2	1010430-97-6	32
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	1,3-Dioxolane, 2-ethyl-	102	C5H10O2	002568-96-9	10





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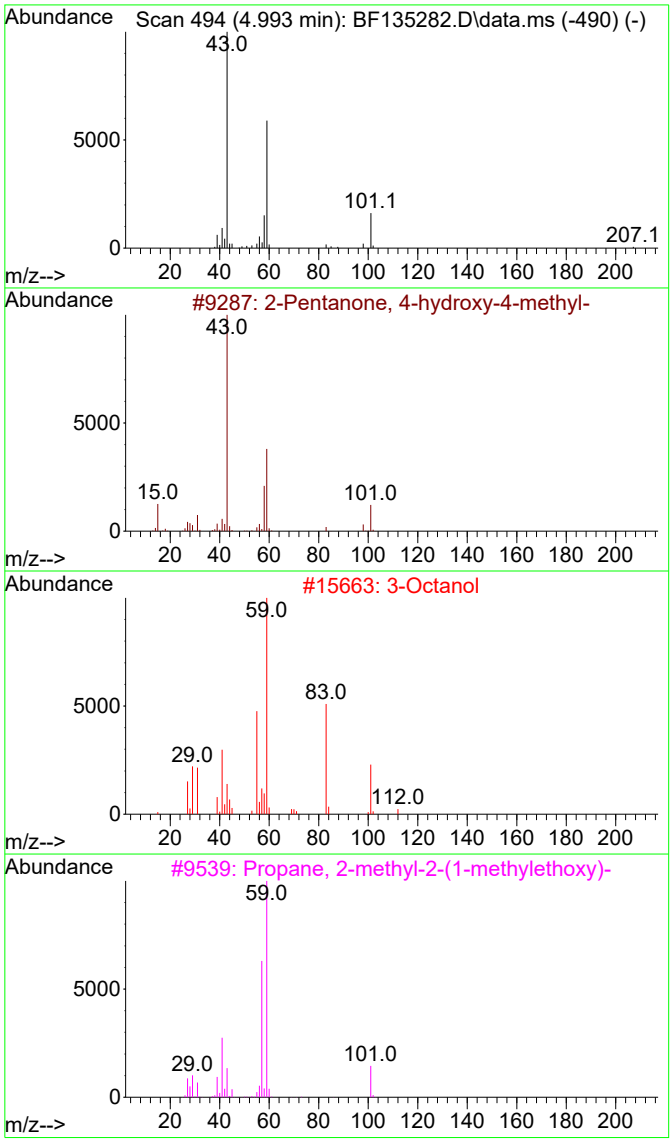
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

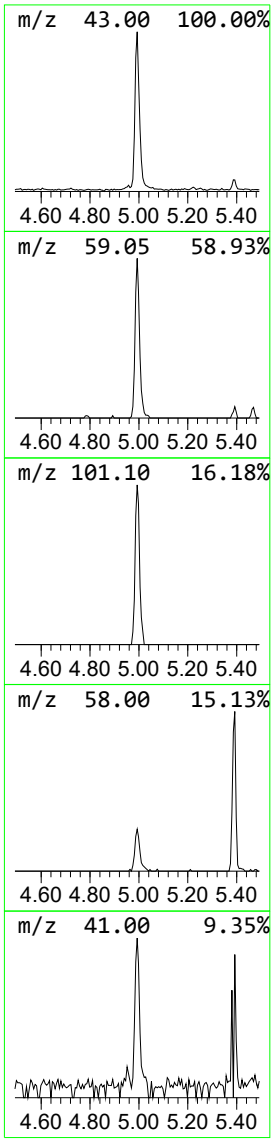
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.993	2.51 ng	84342	1,4-Dichlorobenzene-d4	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	3-Octanol	130	C8H18O	000589-98-0	36
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25





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ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-3(0-2)COMP

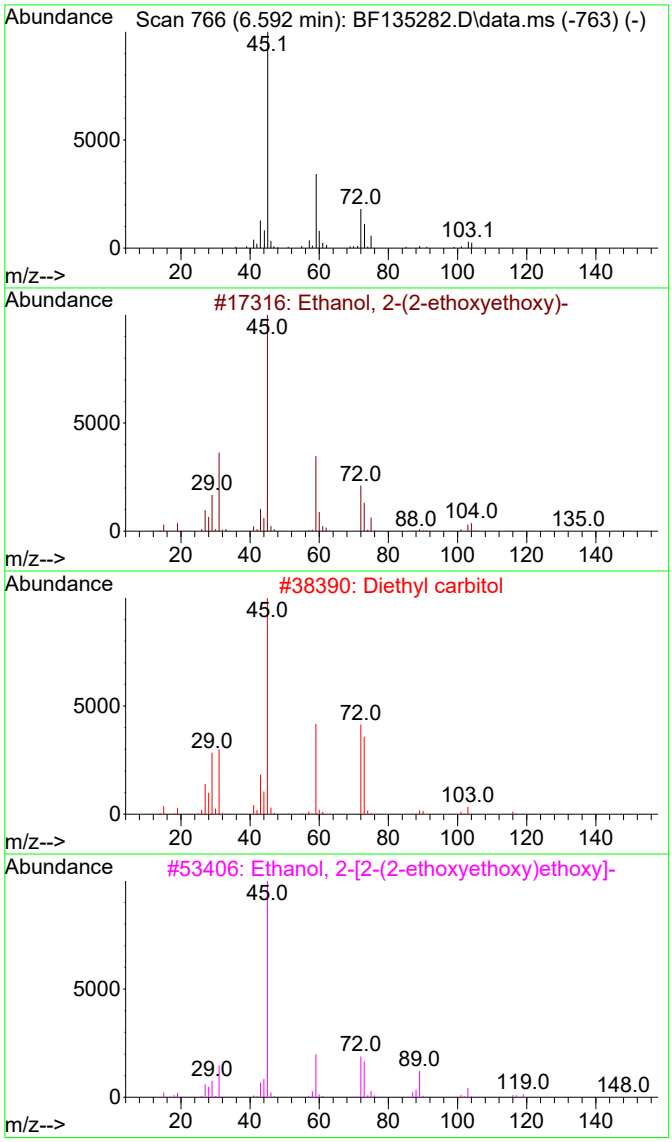
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

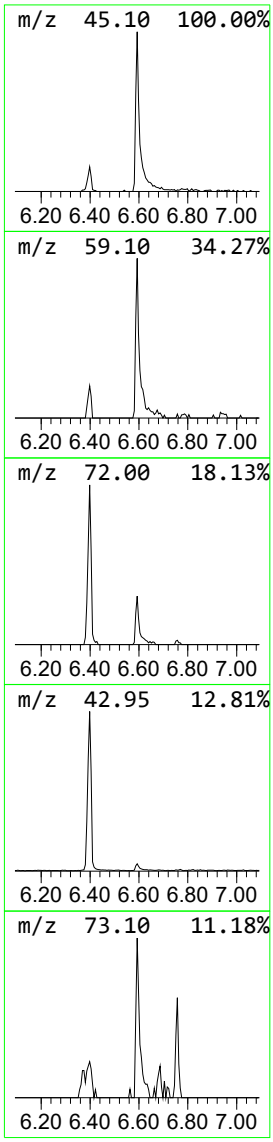
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.592	2.21 ng	74447	1,4-Dichlorobenzene-d4	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2	Diethyl carbitol	162	C8H18O3	000112-36-7	78
3	Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	50
4	Acetic acid, hydroxy-, ethyl ester	104	C4H8O3	000623-50-7	45
5	2-Propanol, 1-propoxy-	118	C6H14O2	001569-01-3	39





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

TIC Library : C:\Database\NIST20.L
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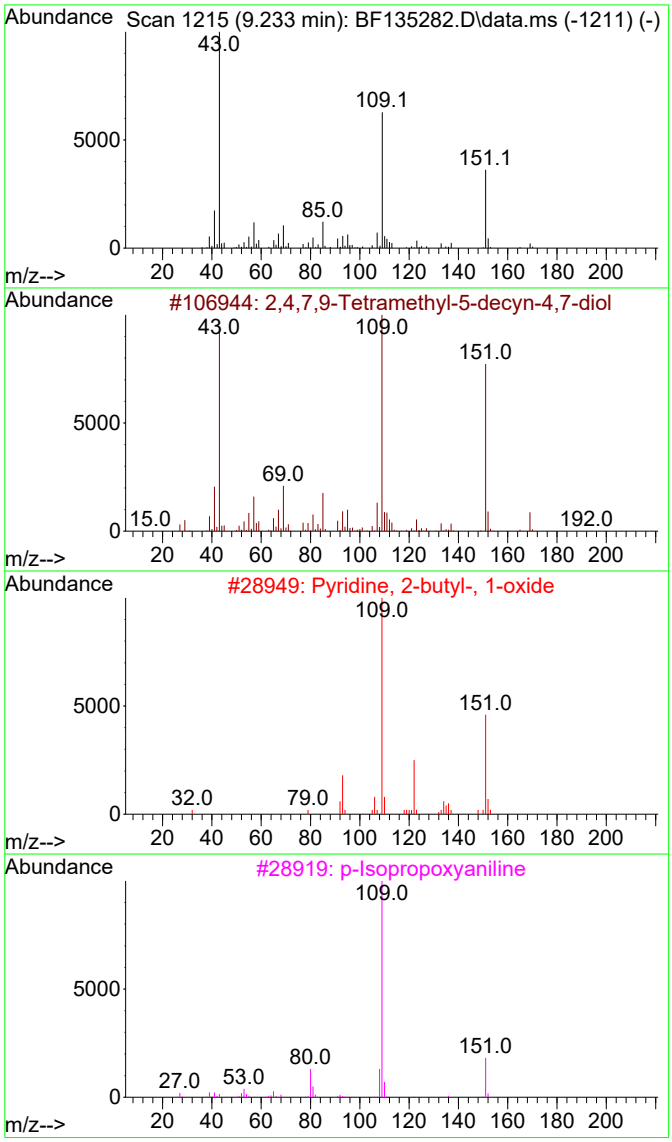
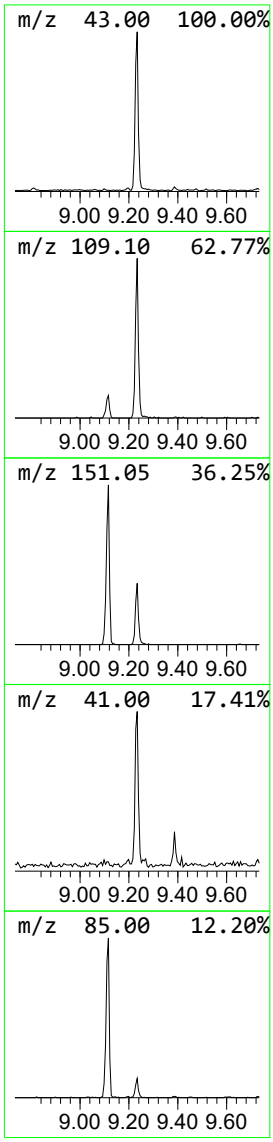
****
Peak Number 4 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.233	3.87 ng	168987	Acenaphthene-d10	9.792

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	87
2	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	53
3	p-Isopropoxyaniline	151	C9H13NO	007664-66-6	49
4	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	47
5	Metacetamol	151	C8H9NO2	000621-42-1	47





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

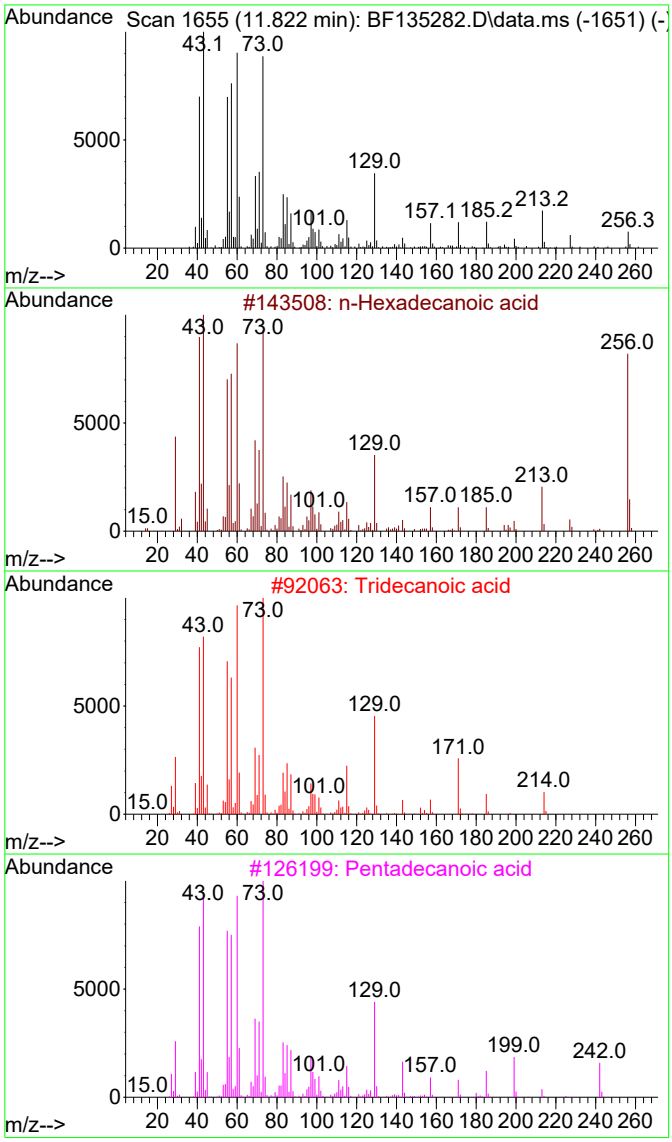
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

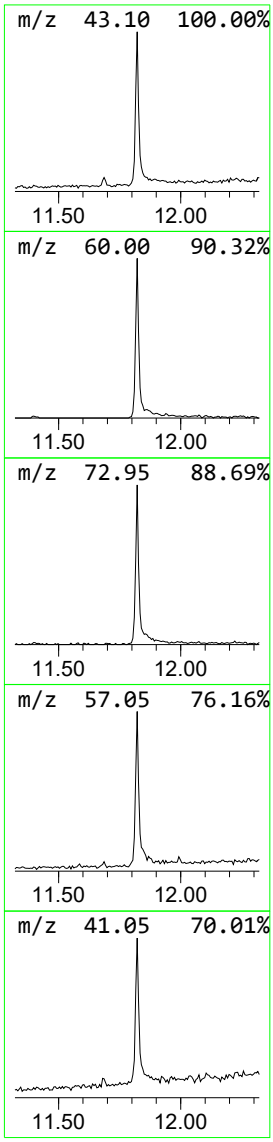
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.822	8.68 ng	336029	Phenanthrene-d10	11.286

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	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5	Dodecanoic acid	200	C12H24O2	000143-07-7	81





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ClientSampleId :
WC-3(0-2)COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

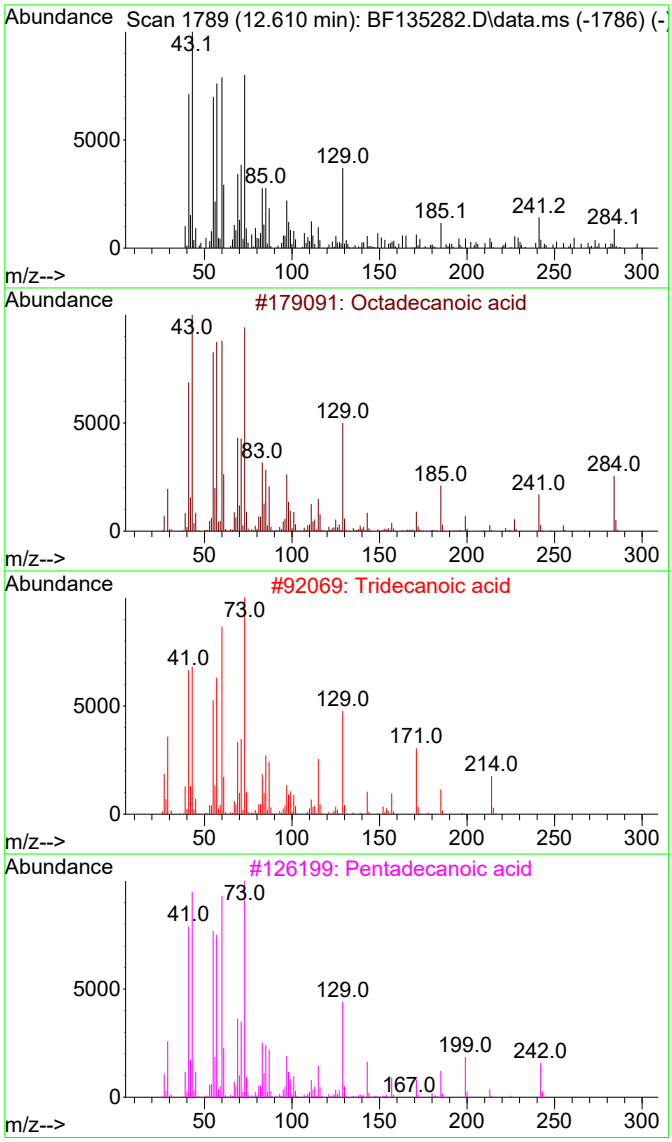
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

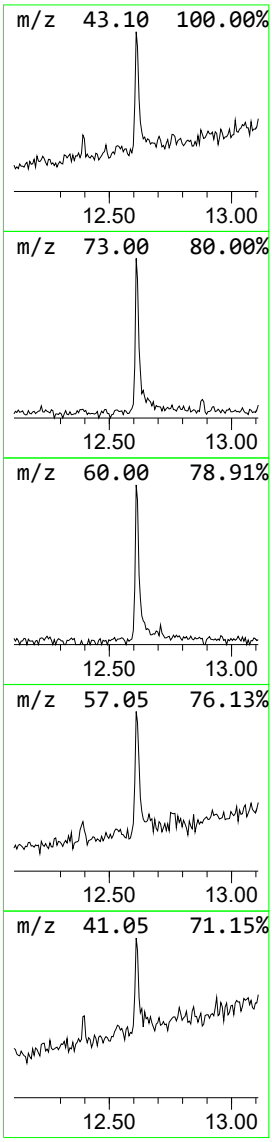
****

Peak Number 6 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.610	3.26 ng	126399	Phenanthrene-d10	11.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
5	n-Decanoic acid	172	C10H20O2	000334-48-5	60





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

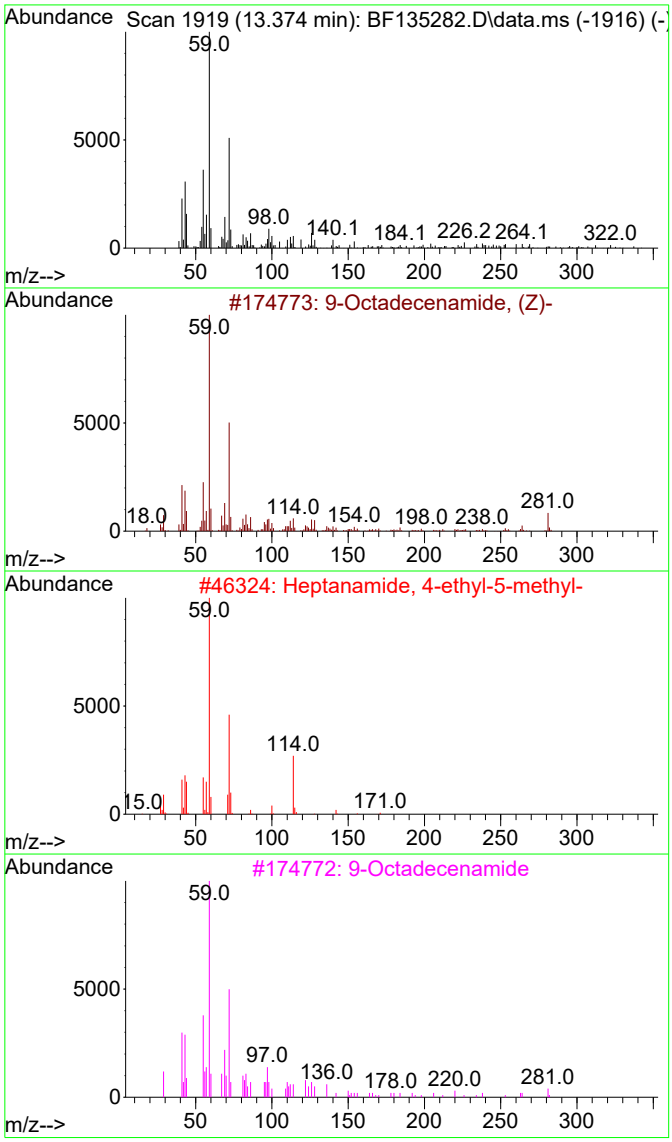
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

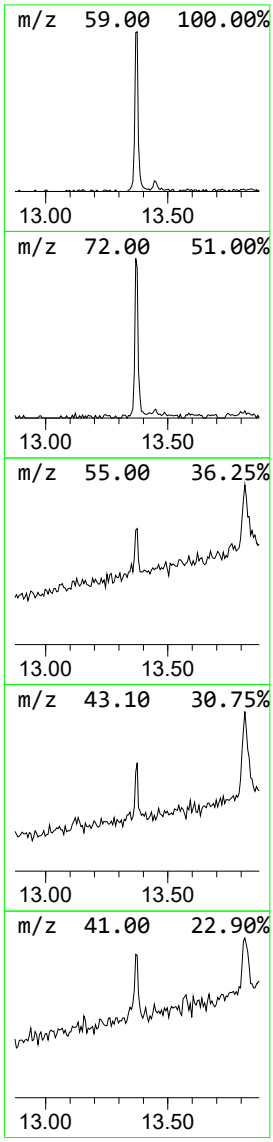
****

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.374	3.14 ng	93175	Chrysene-d12	13.945

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	93
2	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	80
3	9-Octadecenamide	281	C18H35NO	003322-62-1	78
4	7-Nonenamide	155	C9H17NO	090949-53-4	72
5	Tetradecanamide	227	C14H29NO	000638-58-4	64





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propane, 1,1-di...	2.122	2.1	ng	71097	1	6.757	672919	20.0
2-Pentanone, 4-...	4.993	2.5	ng	84342	1	6.757	672919	20.0
Ethanol, 2-(2-e...	6.592	2.2	ng	74447	1	6.757	672919	20.0
2,4,7,9-Tetrame...	9.233	3.9	ng	168987	3	9.792	872363	20.0
n-Hexadecanoic ...	11.822	8.7	ng	336029	4	11.286	774703	20.0
Octadecanoic acid	12.610	3.3	ng	126399	4	11.286	774703	20.0
9-Octadecenamid...	13.374	3.1	ng	93175	5	13.945	593948	20.0