LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091021\
Data File : BF125423.D
Acq On : 10 Sep 2021 14:40
Operator : JU/CG
Sample : M3688-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A688

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-BF081821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125423.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.181	8	16	22	rVB	3109840	4137440	91.52%	14.041%
2	5.098	509	512	523	rVB	167453	189523	4.19%	0.643%
3	5.510	578	582	595	rBV	1991986	1816970	40.19%	6.166%
4	6.510	749	752	760	rBV	1064052	1075717	23.79%	3.651%
5	6.887	812	816	819	rBV	962161	827376	18.30%	2.808%
6	7.451	906	912	915	rBV	2685502	2642615	58.45%	8.968%
7	8.081	1013	1019	1022	rBV2	36762	64781	1.43%	0.220%
8	8.169	1030	1034	1037	rBV	1136159	1053157	23.29%	3.574%
9	9.245	1212	1217	1220	rBV	5045748	4521050	100.00%	15.343%
10	9.586	1271	1275	1280	rBV2	87491	113344	2.51%	0.385%
11	9.827	1312	1316	1321	rBV8	31198	51910	1.15%	0.176%
12	9.922	1328	1332	1336	rBV	1280172	1192157	26.37%	4.046%
13	10.327	1395	1401	1408	rBV9	37901	71626	1.58%	0.243%
14	10.716	1463	1467	1476	rBV	3066478	3019069	66.78%	10.246%
15	11.416	1582	1586	1589	rVB	1241113	1140835	25.23%	3.872%
16	11.933	1670	1674	1677	rBV2	367365	350617	7.76%	1.190%
17	12.716	1804	1807	1819	rVB	148029	175587	3.88%	0.596%
18	13.004	1851	1856	1859	rVB	4829546	4488615	99.28%	15.233%
19	13.880	2001	2005	2008	rBV3	109475	144045	3.19%	0.489%
20	13.921	2008	2012	2025	rVB2	163412	286795	6.34%	0.973%
21	14.057	2031	2035	2040	rVB	1152966	946143	20.93%	3.211%
22	14.686	2138	2142	2148	rVB	124030	165739	3.67%	0.562%
23	15.551	2283	2289	2294	rBV	684346	885793	19.59%	3.006%
24	15.633	2299	2303	2310	rVB2	62948	105669	2.34%	0.359%

Sum of corrected areas: 29466573

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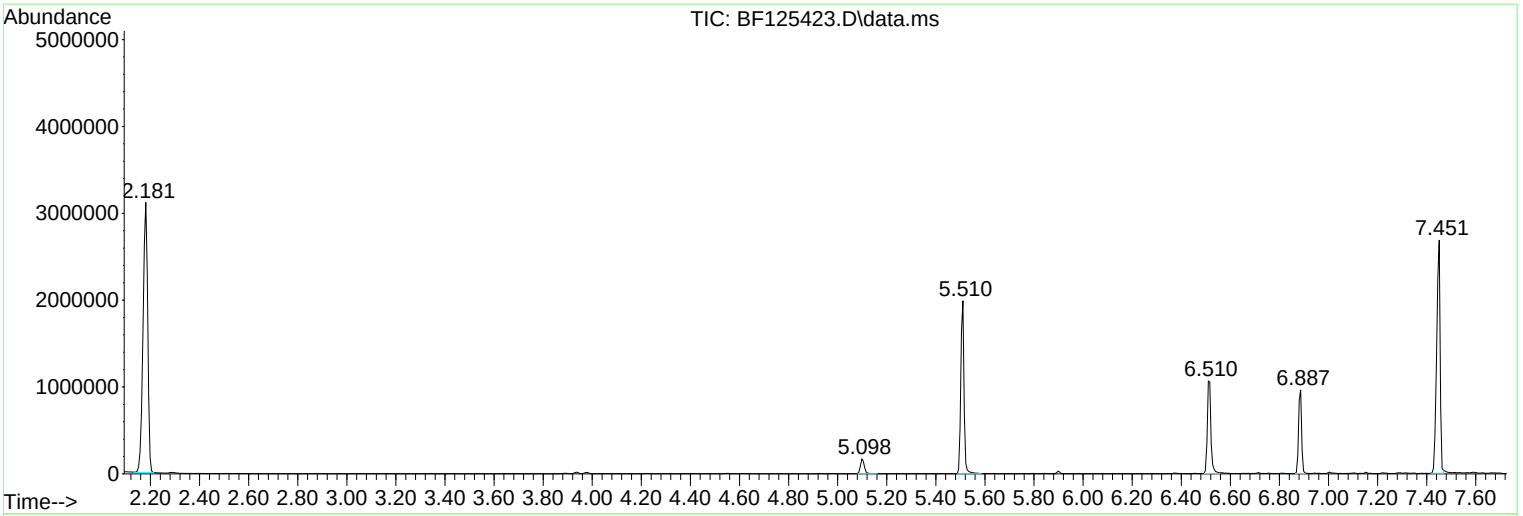
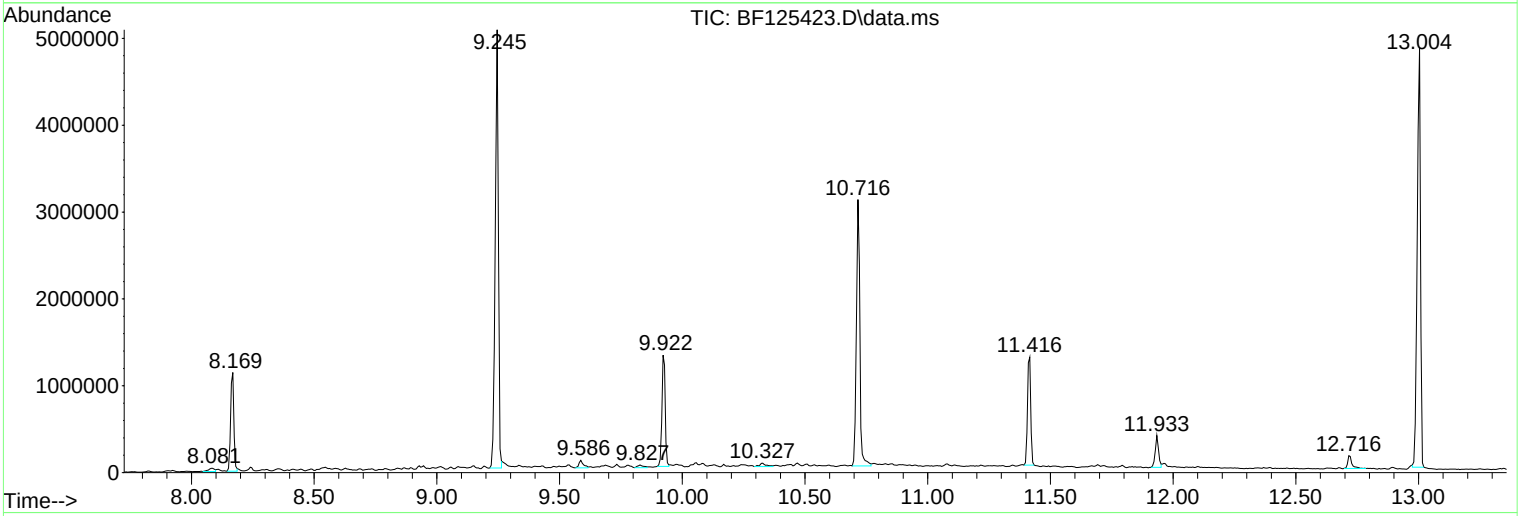
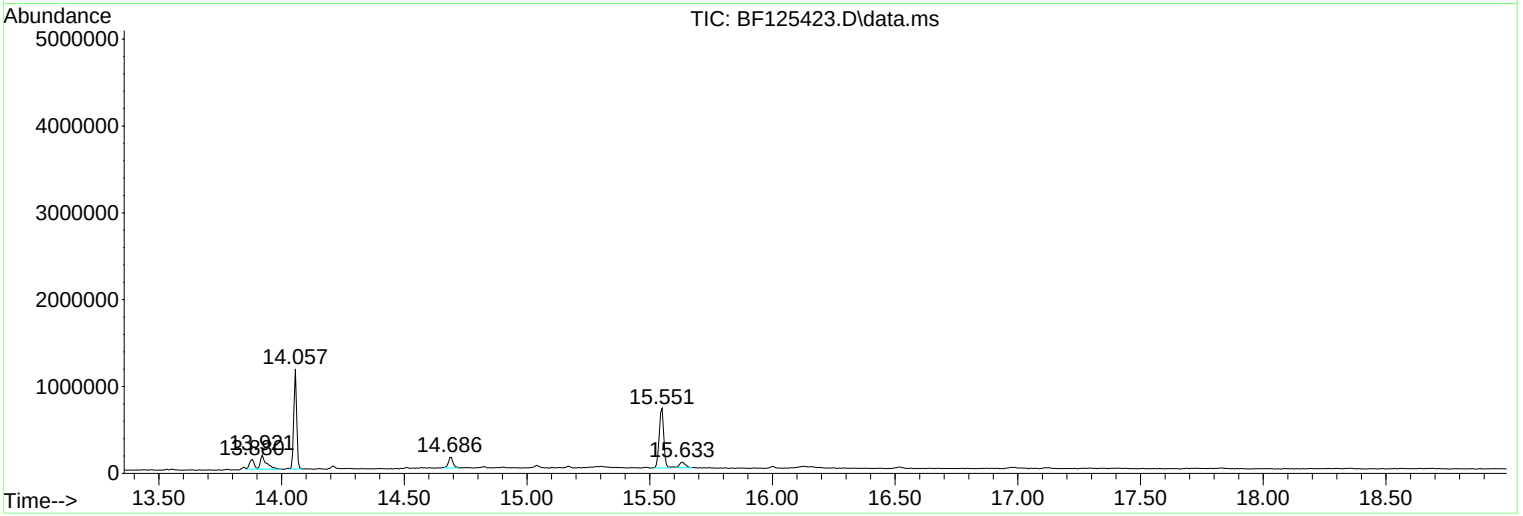
Instrument :
BNA_F
ClientSampleId :
A688

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.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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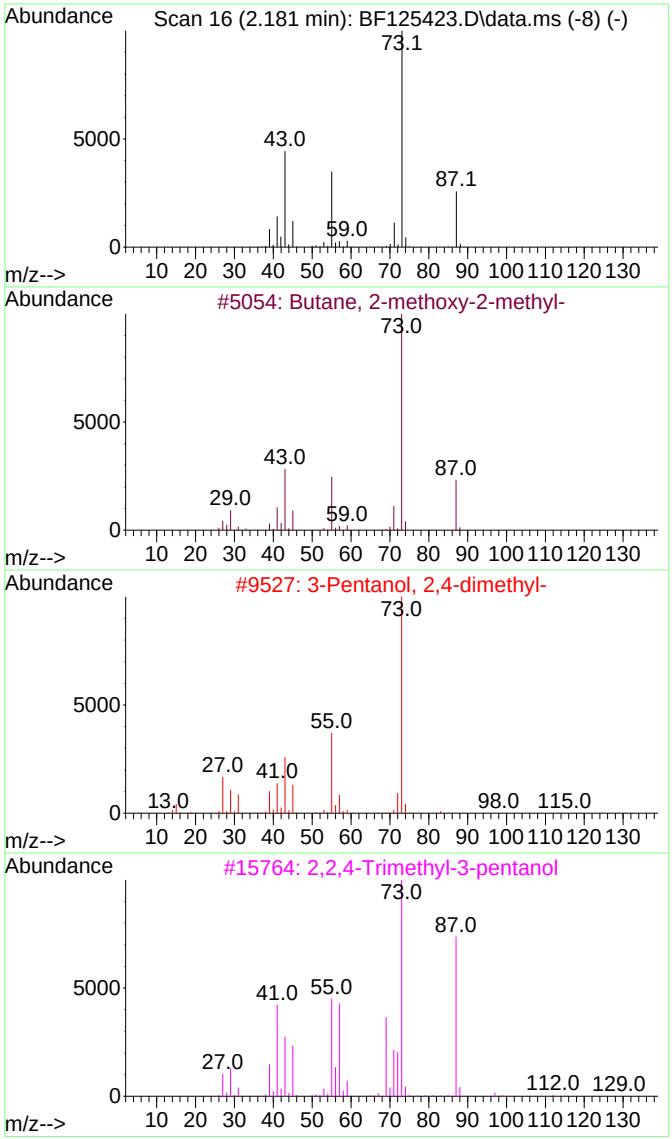
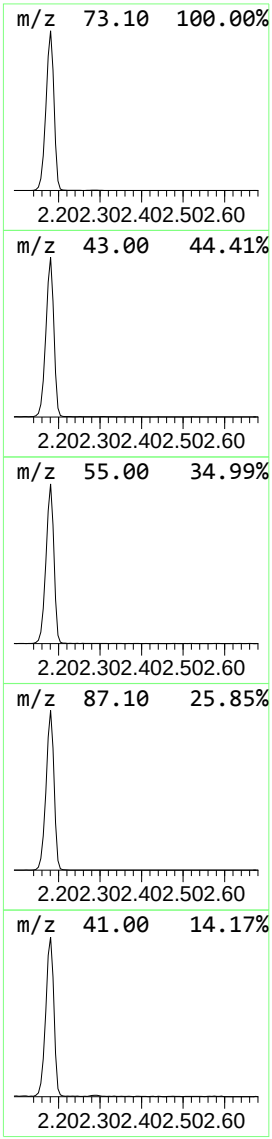
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.181	100.01 ng	4137440	1,4-Dichlorobenzene-d4	6.886

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	23





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Data File : BF125423.D
Acq On : 10 Sep 2021 14:40
Operator : JU/CG
Sample : M3688-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A688

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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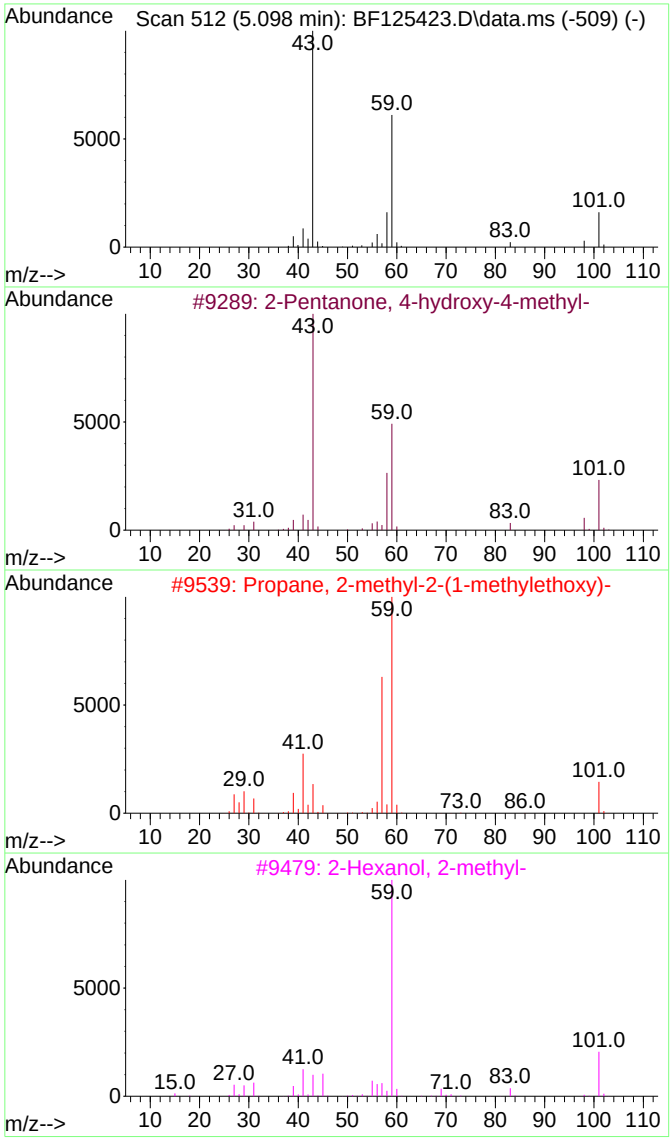
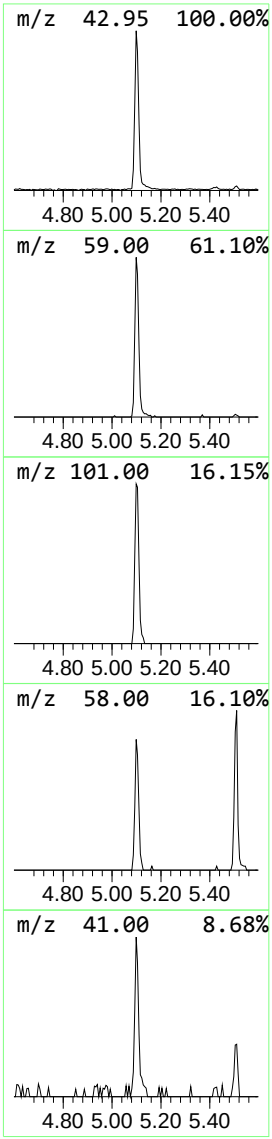
****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.098	4.58 ng	189523	1,4-Dichlorobenzene-d4	6.886

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





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Operator : JU/CG
Sample : M3688-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A688

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
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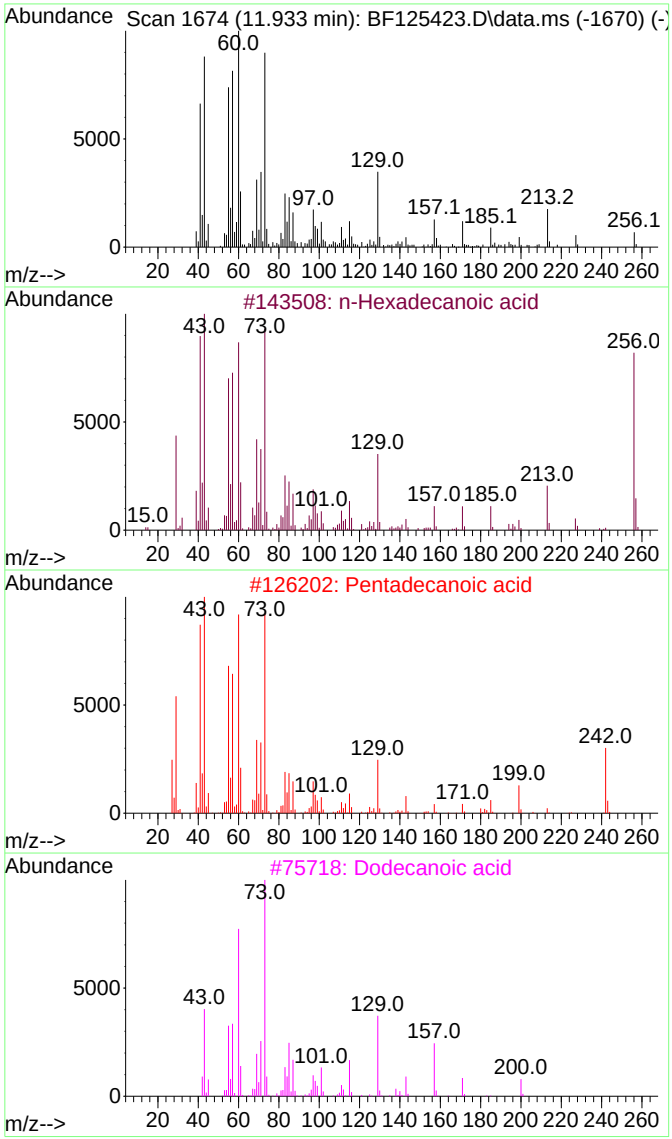
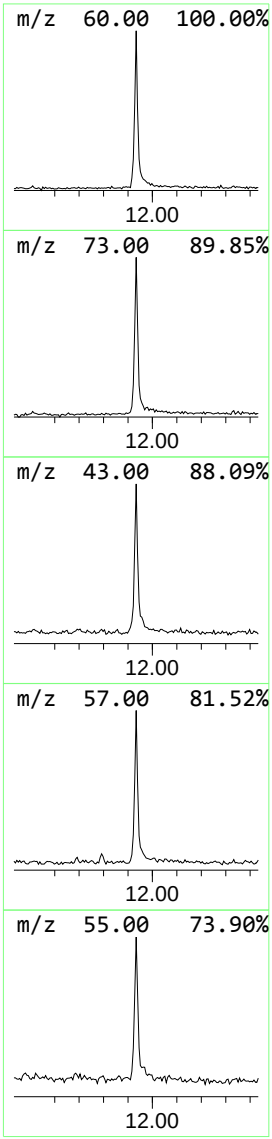
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	6.15 ng	350617	Phenanthrene-d10	11.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3	Dodecanoic acid	200	C12H24O2	000143-07-7	72
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Tridecanoic acid	214	C13H26O2	000638-53-9	70





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Operator : JU/CG
Sample : M3688-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A688

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

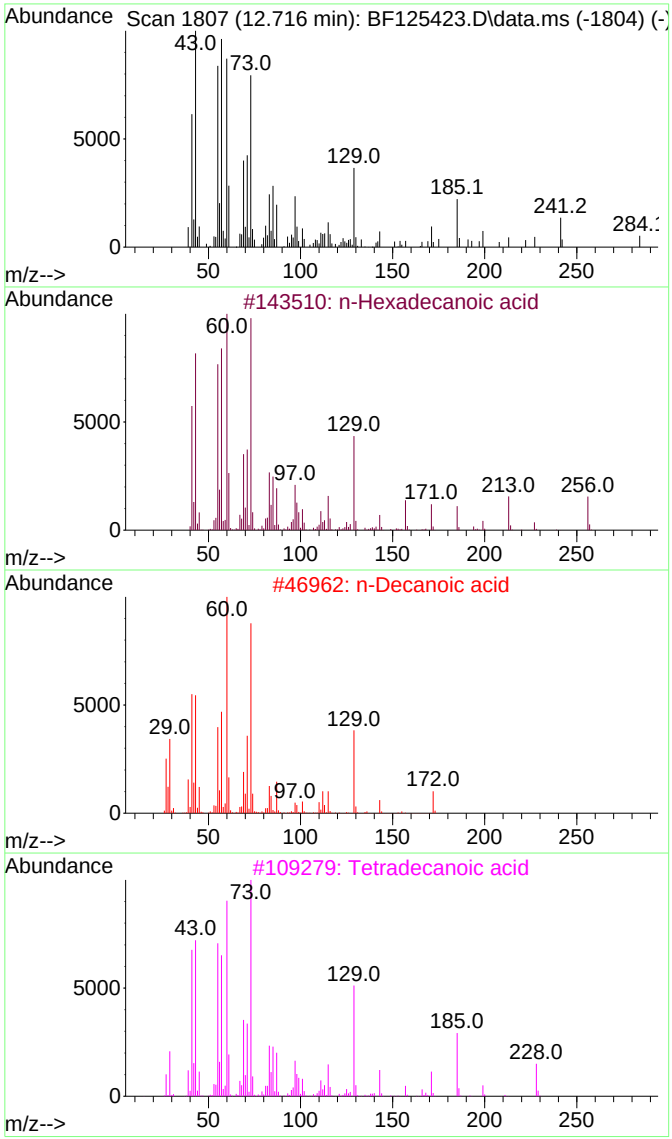
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

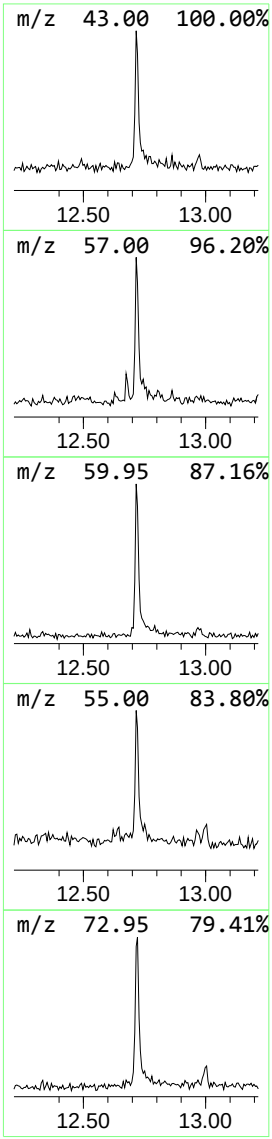
****

Peak Number 4 n-Decanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.716	3.08 ng	175587	Phenanthrene-d10	11.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
2	n-Decanoic acid	172	C10H20O2	000334-48-5	62
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	50
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	43





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Sample : M3688-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A688

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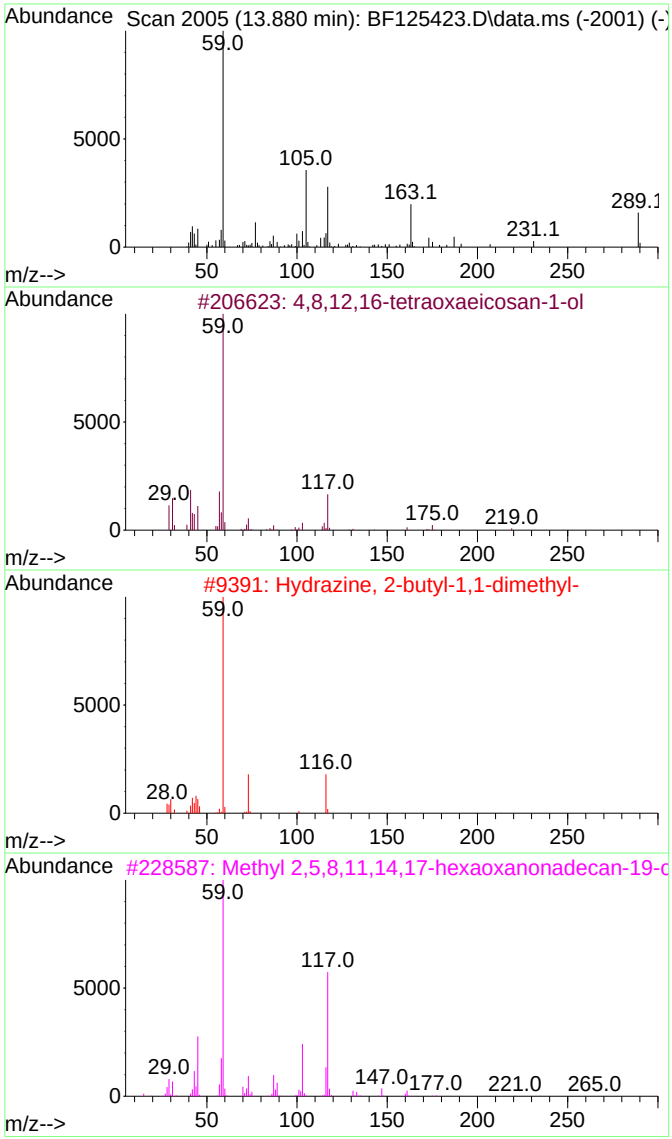
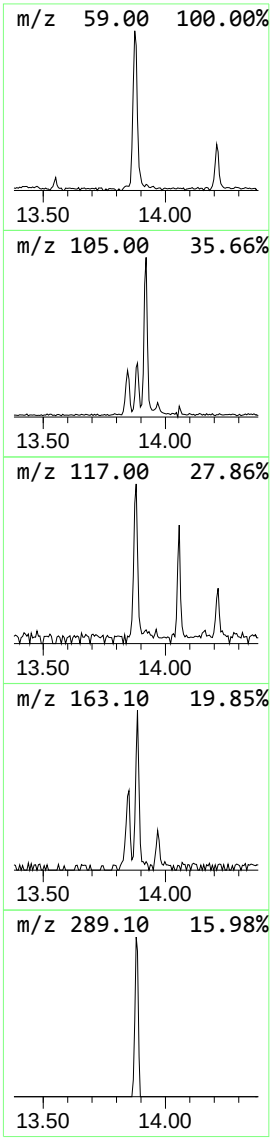
****

Peak Number 5 unknown13.880 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	3.04 ng	144045	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,8,12,16-tetraoxaeicosan-1-ol	306	C16H34O5	1010397-63-6	43
2	Hydrazine, 2-butyl-1,1-dimethyl-	116	C6H16N2	054007-23-7	38
3	Methyl 2,5,8,11,14,17-hexaoxanon...	324	C14H28O8	1000366-81-4	38
4	Methyl 2,5,8,11,14,17,20,23,26-n...	456	C20H40O11	1000366-81-1	38
5	1-Propanol, 2-(2-methoxypropoxy)-	148	C7H16O3	013588-28-8	37





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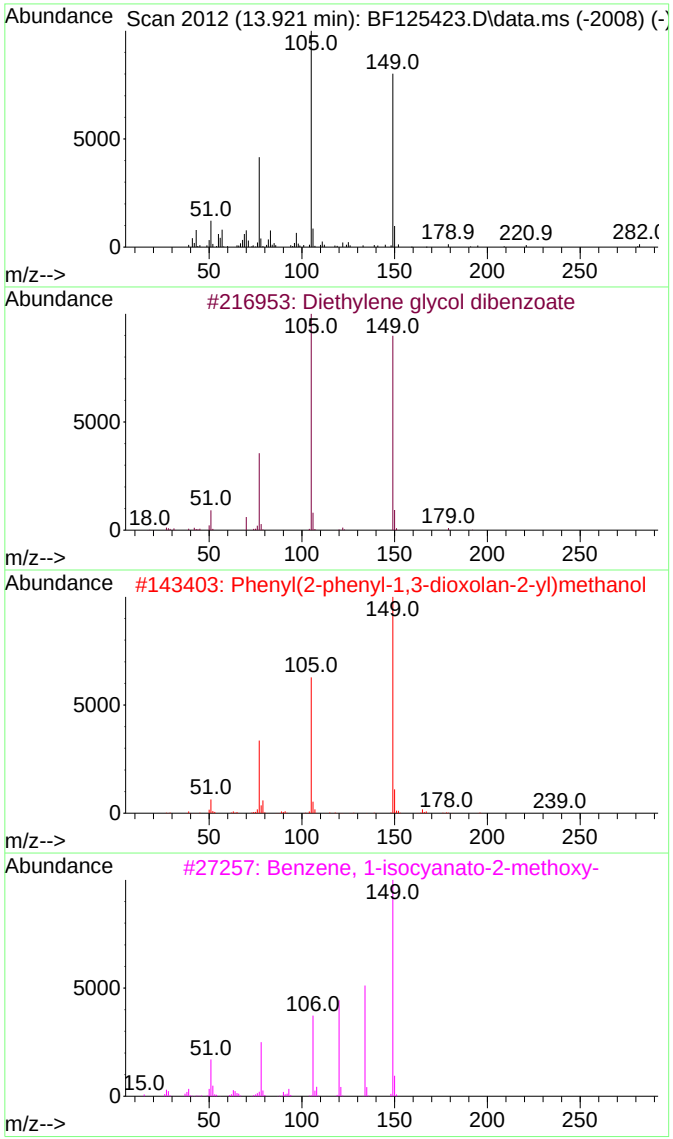
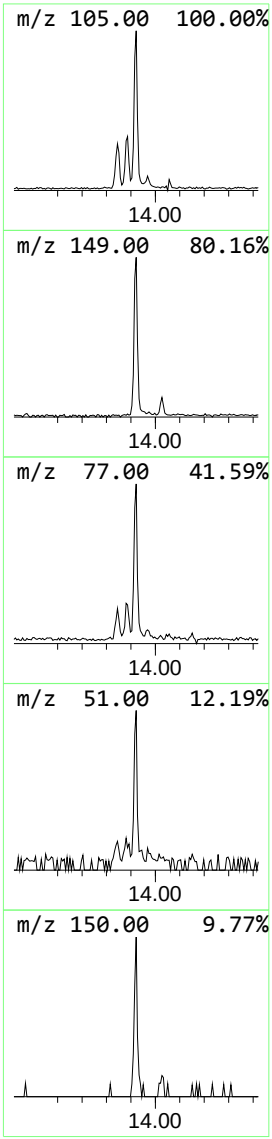
****
Peak Number 6 Diethylene glycol dibenzoate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.921	6.06 ng	286795	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	90
2	Phenyl(2-phenyl-1,3-dioxolan-2-y...	256	C16H16O3	005694-69-9	72
3	Benzene, 1-isocyanato-2-methoxy-	149	C8H7NO2	000700-87-8	46
4	Phthalic acid, 7-bromoheptyl oct...	454	C23H35BrO4	1000415-52-2	43
5	Phthalic acid, propyl octadecyl ...	460	C29H48O4	1000308-96-7	38





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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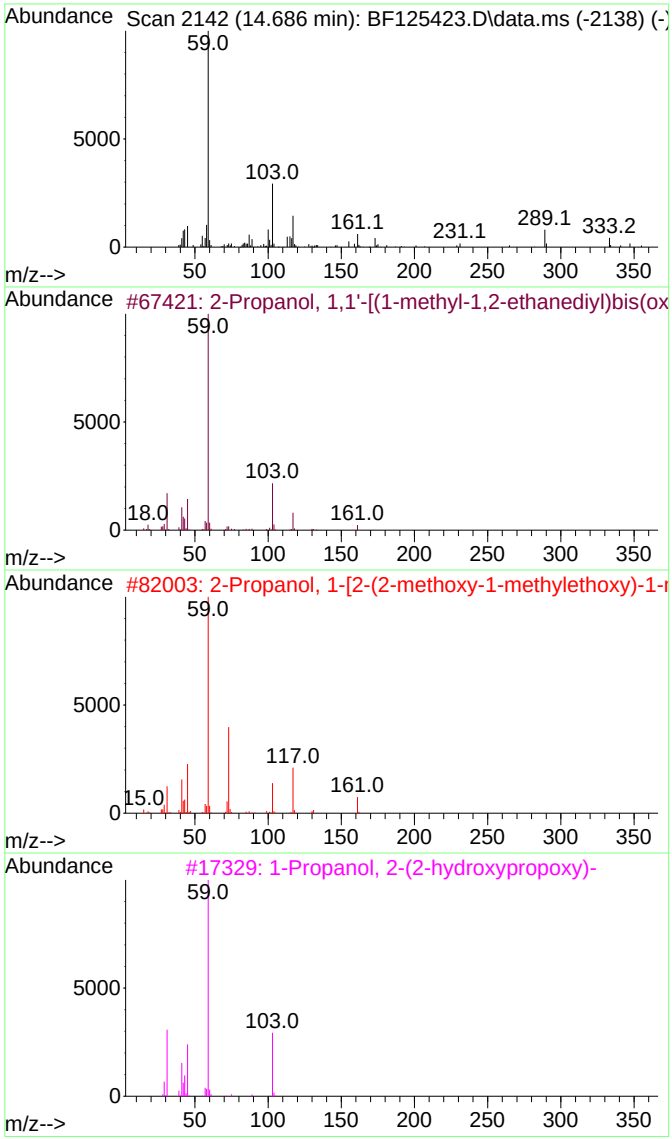
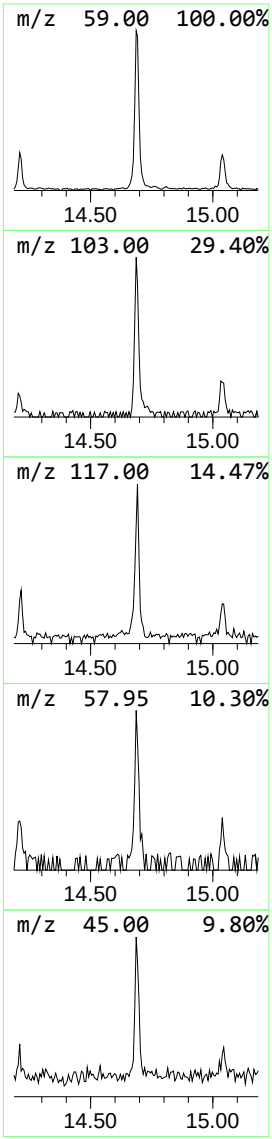
****
Peak Number 7 2-Propanol, 1,1'-[(1-methyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.686	3.50 ng	165739	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1,1'-[(1-methyl-1,2-...	192	C9H20O4	001638-16-0	64
2	2-Propanol, 1-[2-(2-methoxy-1-me...	206	C10H22O4	020324-33-8	59
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	53
4	1-(1-tert-Butoxypropan-2-yloxy)p...	190	C10H22O3	132739-31-2	53
5	Allyldimethylsilane	100	C5H12Si	003937-30-2	43





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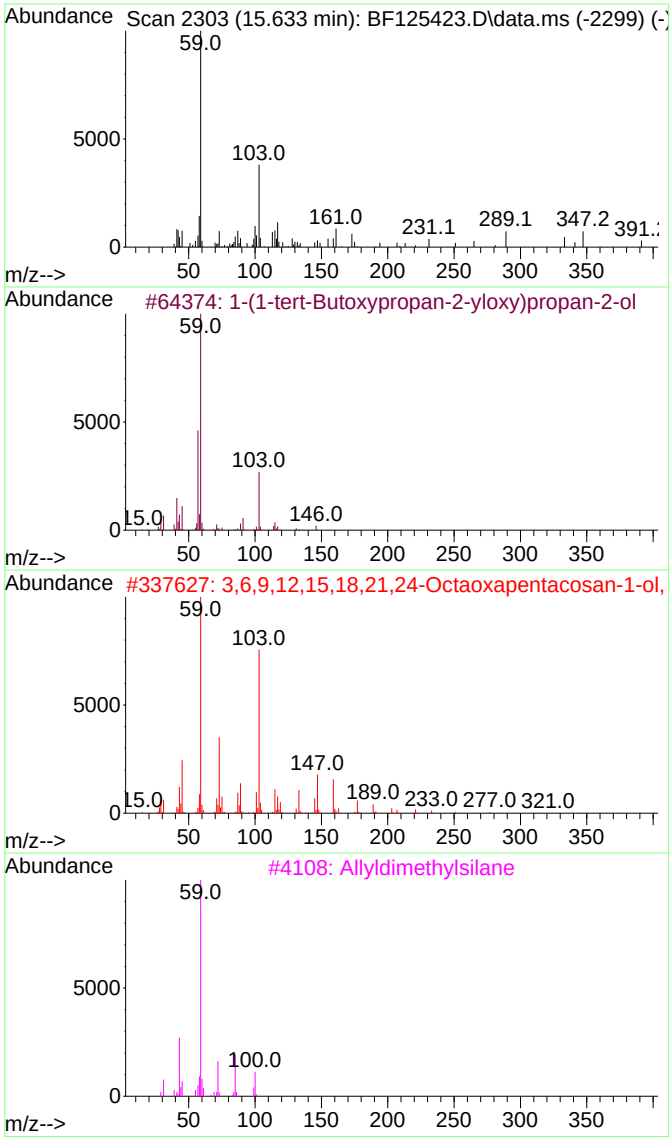
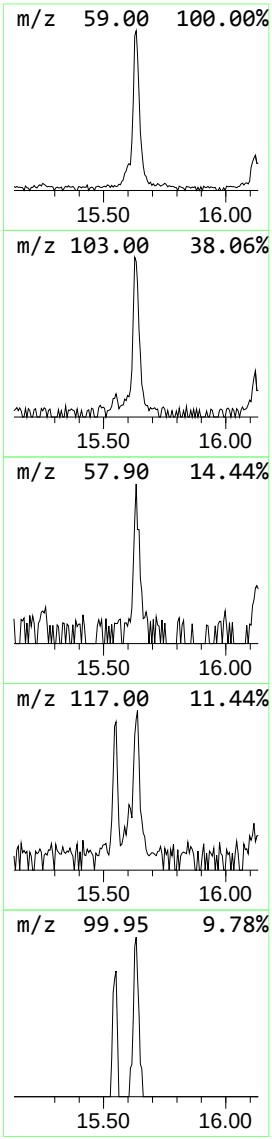
****
Peak Number 8 1-(1-tert-Butoxypropan-2-yl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.633	2.39 ng	105669	Perylene-d12	15.551

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(1-tert-Butoxypropan-2-yloxy)p...	190	C10H22O3	132739-31-2	59
2	3,6,9,12,15,18,21,24-Octaoxapent...	498	C23H50O9Si	1000352-09-8	45
3	Allyldimethylsilane	100	C5H12Si	003937-30-2	43
4	2,5,8,11,14,17-Hexaoxaoctadecane	266	C12H26O6	001191-87-3	42
5	Methane, diethoxy-	104	C5H12O2	000462-95-3	42





Tentatively Identified Compound (LSC) summary

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Operator : JU/CG
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
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
Butane, 2-metho...	2.181	100.0	ng	4137440	1	6.886	827376	20.0
2-Pentanone, 4-...	5.098	4.6	ng	189523	1	6.886	827376	20.0
n-Hexadecanoic ...	11.933	6.2	ng	350617	4	11.416	1140840	20.0
n-Decanoic acid	12.716	3.1	ng	175587	4	11.416	1140840	20.0
unknown13.880	13.880	3.0	ng	144045	5	14.057	946143	20.0
Diethylene glyc...	13.921	6.1	ng	286795	5	14.057	946143	20.0
2-Propanol, 1,1...	14.686	3.5	ng	165739	5	14.057	946143	20.0
1-(1-tert-Butox...	15.633	2.4	ng	105669	6	15.551	885793	20.0