LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052021\
Data File : BF124013.D
Acq On : 20 May 2021 17:18
Operator : JU/CG
Sample : M2462-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WATER-MAIN-BREAK-SOIL

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-BF051421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124013.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	4	10	16	rVB	543305	659104	45.56%	5.852%
2	2.257	24	29	34	rVB	37366	47756	3.30%	0.424%
3	5.116	511	515	522	rVB	108558	130229	9.00%	1.156%
4	5.522	579	584	587	rBV	1238201	1118367	77.30%	9.930%
5	6.528	750	755	758	rBV	1223076	1163857	80.44%	10.334%
6	6.904	816	819	823	rBV	395829	300883	20.80%	2.672%
7	7.469	910	915	918	rBV	879599	784337	54.21%	6.964%
8	8.192	1034	1038	1041	rBV	474527	397967	27.51%	3.534%
9	9.263	1216	1220	1223	rBV	1706572	1446810	100.00%	12.846%
10	9.375	1237	1239	1242	rBV	30990	29083	2.01%	0.258%
11	9.657	1284	1287	1291	rBV2	40668	41310	2.86%	0.367%
12	9.945	1332	1336	1340	rBV	649926	494463	34.18%	4.390%
13	10.733	1466	1470	1473	rBV	1141851	948734	65.57%	8.424%
14	10.863	1490	1492	1500	rVB2	18266	19101	1.32%	0.170%
15	11.298	1562	1566	1568	rBV4	14592	16289	1.13%	0.145%
16	11.433	1585	1589	1591	rBV	582238	470346	32.51%	4.176%
17	11.457	1591	1593	1597	rVB	40389	34422	2.38%	0.306%
18	11.951	1675	1677	1683	rBV2	74072	83903	5.80%	0.745%
19	12.521	1770	1774	1778	rBV5	11138	16824	1.16%	0.149%
20	12.645	1792	1795	1798	rBV	119660	95282	6.59%	0.846%
21	12.874	1829	1834	1840	rVB3	85253	96026	6.64%	0.853%
22	13.021	1854	1859	1862	rBV	1660508	1357669	93.84%	12.055%
23	13.092	1867	1871	1876	rVB7	10936	17741	1.23%	0.158%
24	13.586	1951	1955	1960	rBV7	16504	26322	1.82%	0.234%
25	13.710	1973	1976	1979	rBV5	18182	18946	1.31%	0.168%
26	13.827	1992	1996	1999	rVB6	14352	21026	1.45%	0.187%
27	13.915	2008	2011	2019	rVB	242979	277936	19.21%	2.468%
28	14.074	2033	2038	2041	rBV	449533	451001	31.17%	4.004%
29	14.098	2041	2042	2045	rVB	50189	38089	2.63%	0.338%
30	14.180	2053	2056	2058	rVB4	18516	16250	1.12%	0.144%
31	14.557	2116	2120	2125	rBV8	35052	54319	3.75%	0.482%
32	14.857	2169	2171	2175	rVB4	20391	23800	1.64%	0.211%
33	15.133	2214	2218	2220	rBV2	40627	62479	4.32%	0.555%
34	15.209	2229	2231	2234	rVB4	27967	27798	1.92%	0.247%
35	15.445	2267	2271	2274	rVB2	24535	34756	2.40%	0.309%
36	15.509	2277	2282	2286	rVB4	27455	49957	3.45%	0.444%

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Instrument :
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ClientSampleId :
WATER-MAIN-BREAK-SOIL

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-BF051421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.574	2288	2293	2296	rBV	208091	284221	19.64%	2.524%
38	15.851	2338	2340	2344	rBV5	14045	21994	1.52%	0.195%
39	16.121	2382	2386	2391	rBV8	30533	64362	4.45%	0.571%
40	16.498	2448	2450	2455	rBV6	11031	18740	1.30%	0.166%

Sum of corrected areas: 11262499

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ClientSampleId :
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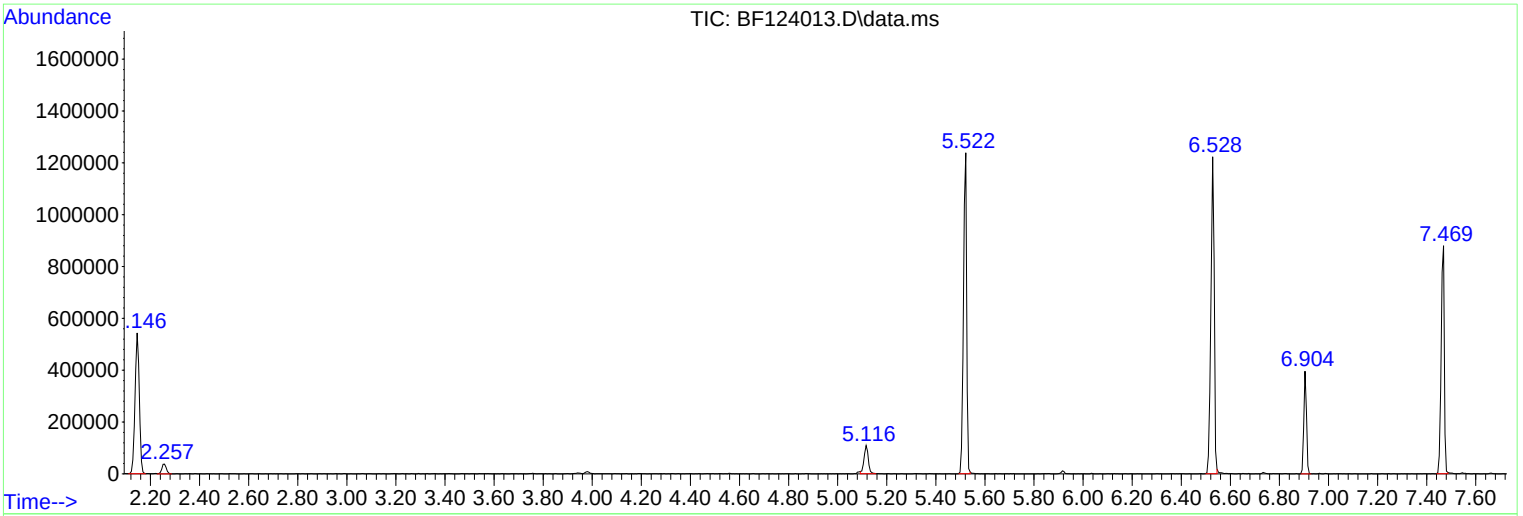
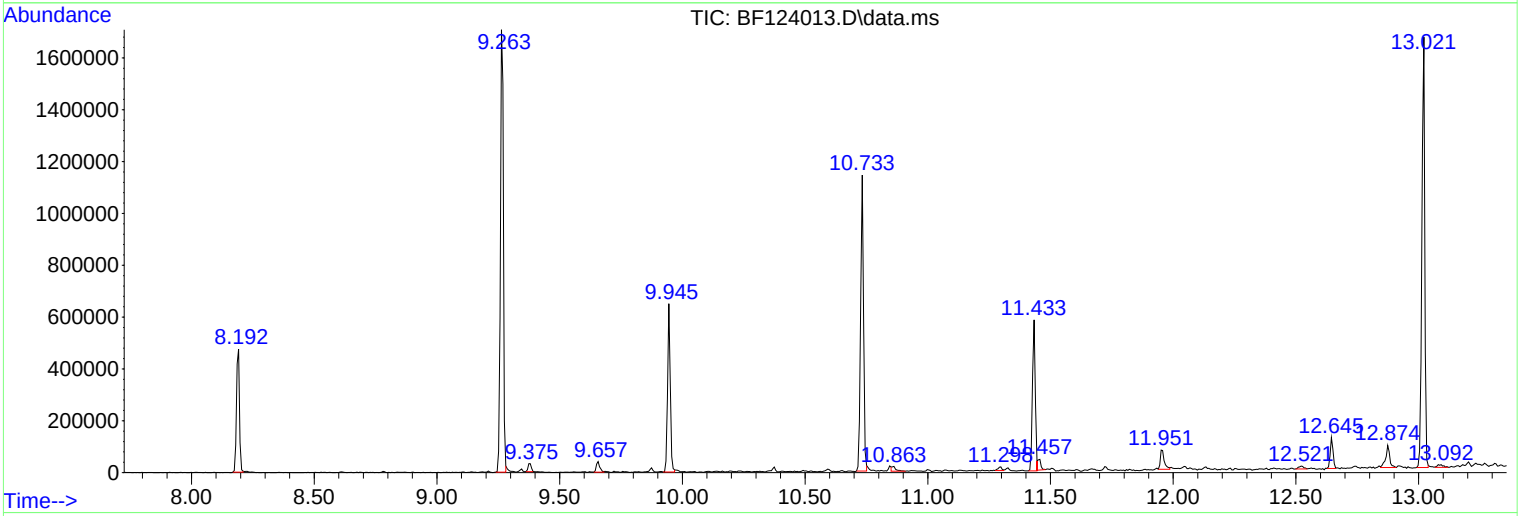
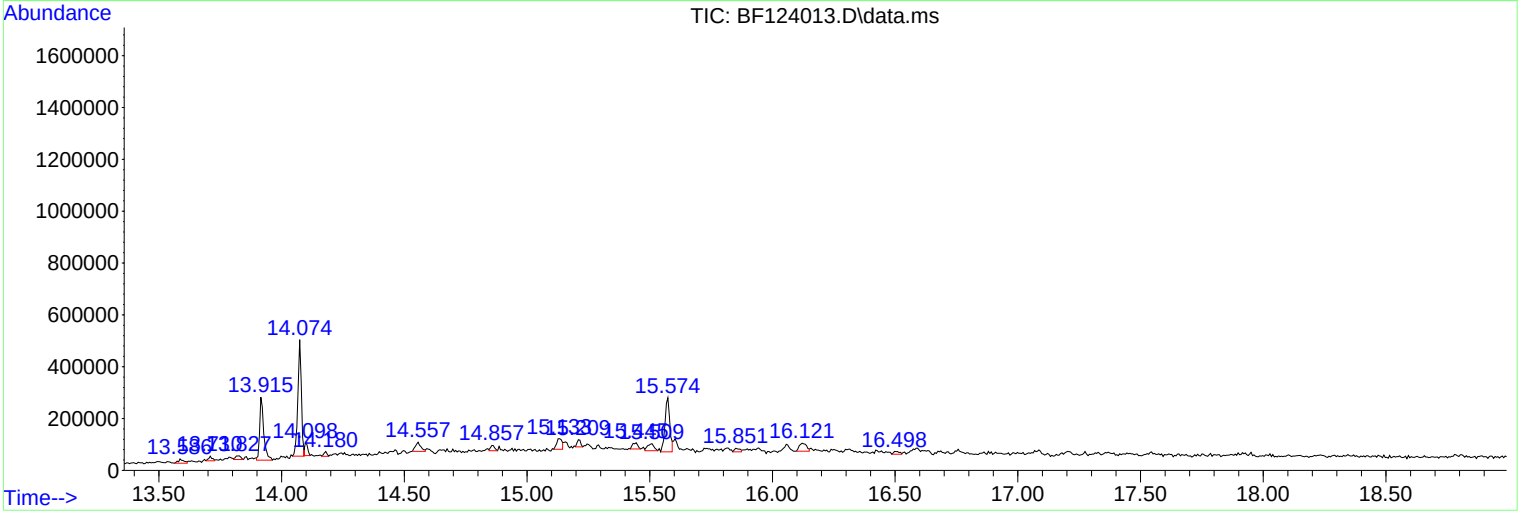
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P







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Data File : BF124013.D
Acq On : 20 May 2021 17:18
Operator : JU/CG
Sample : M2462-01
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ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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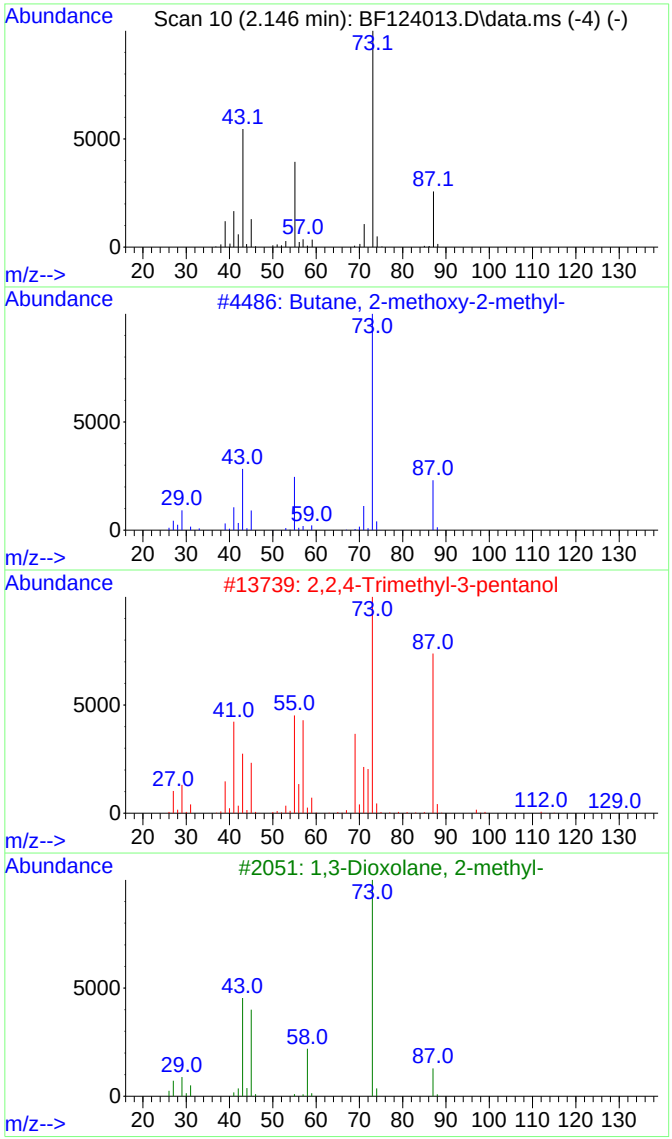
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

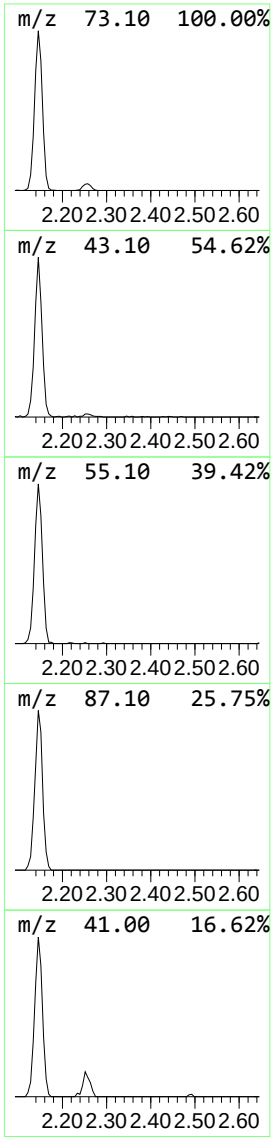
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.146	43.81 ng	659104	1,4-Dichlorobenzene-d4	6.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





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Sample : M2462-01
Misc :
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Instrument :
BNA_F
ClientSampleId :
WATER-MAIN-BREAK-SOIL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

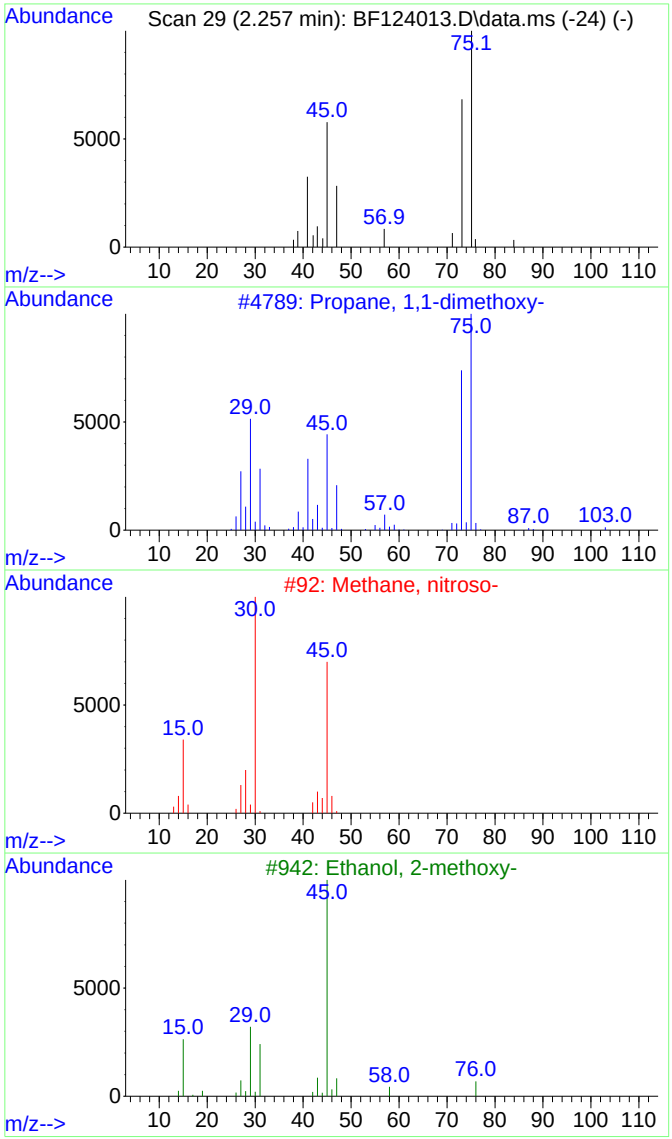
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

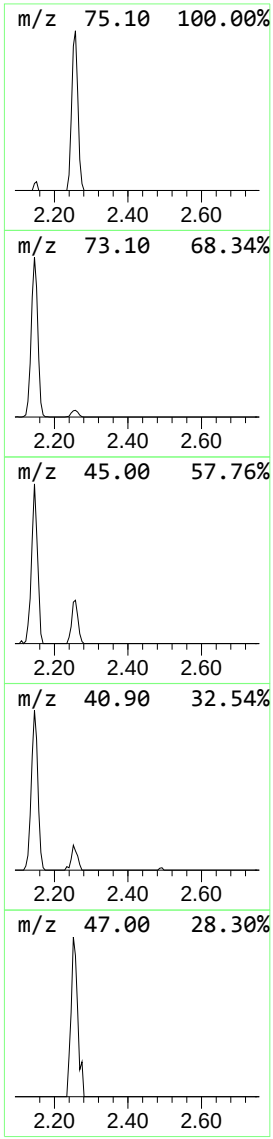
****

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.257	3.17 ng	47756	1,4-Dichlorobenzene-d4	6.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	78
2	Methane, nitroso-	45	CH3NO	000865-40-7	5
3	Ethanol, 2-methoxy-	76	C3H8O2	000109-86-4	5
4	Methylal	76	C3H8O2	000109-87-5	4
5	Glycine	75	C2H5NO2	000056-40-6	4





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Sample : M2462-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WATER-MAIN-BREAK-SOIL

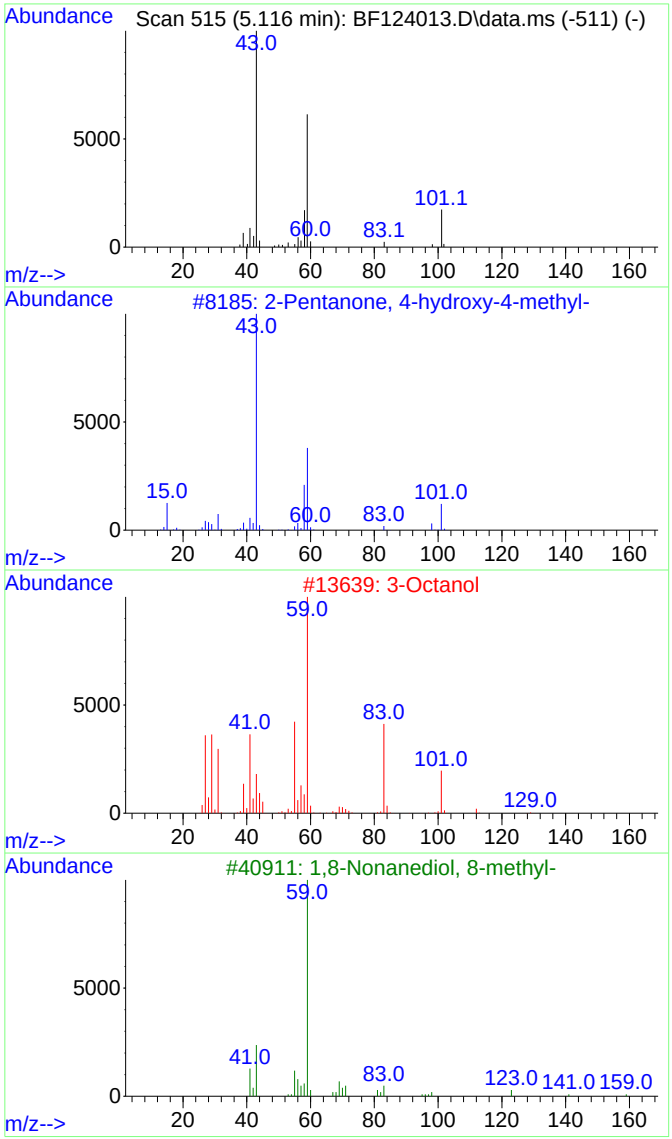
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

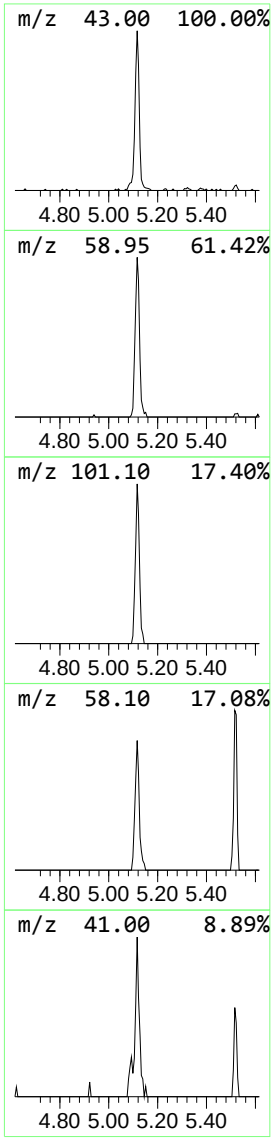
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.116	8.66 ng	130229	1,4-Dichlorobenzene-d4	6.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	3-Octanol	130	C8H18O	000589-98-0	33
3	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

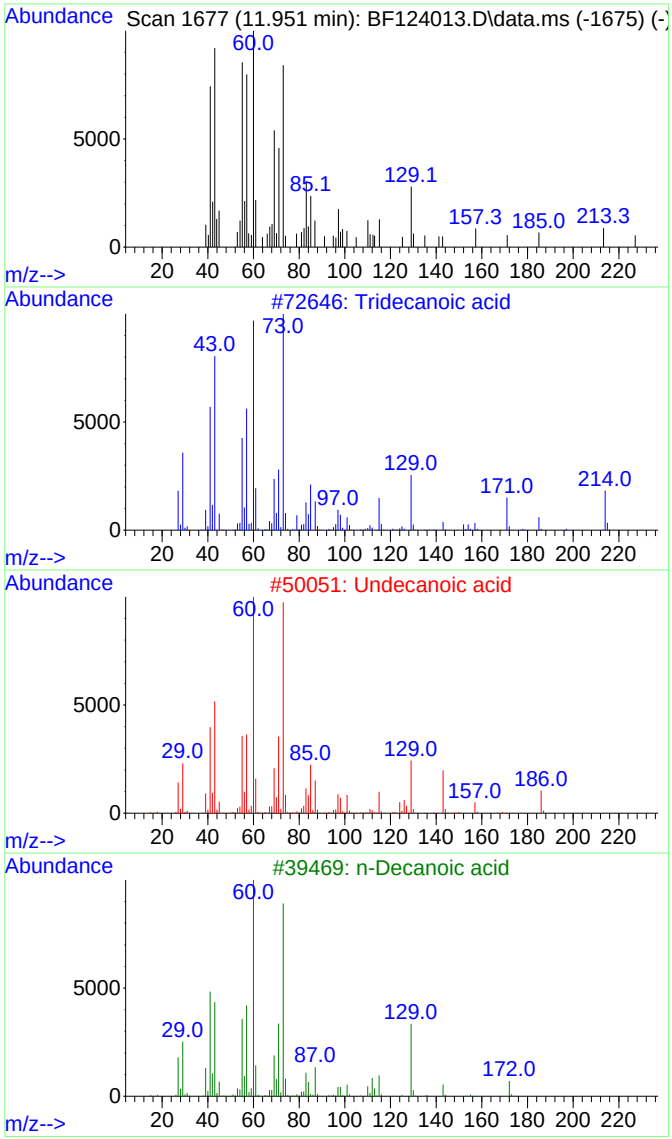
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

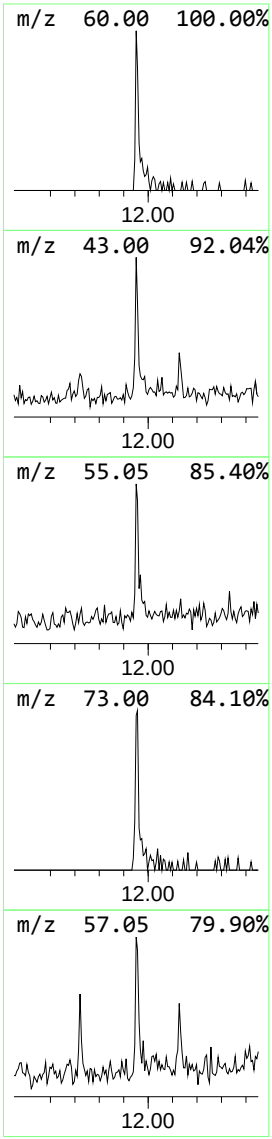
****

Peak Number 4 Tridecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.951	3.57 ng	83903	Phenanthrene-d10	11.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	80
2	Undecanoic acid	186	C11H22O2	000112-37-8	64
3	n-Decanoic acid	172	C10H20O2	000334-48-5	53
4	Dodecanoic acid	200	C12H24O2	000143-07-7	53
5	Silver butanoate	194	C4H7AgO2	005076-24-4	47





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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
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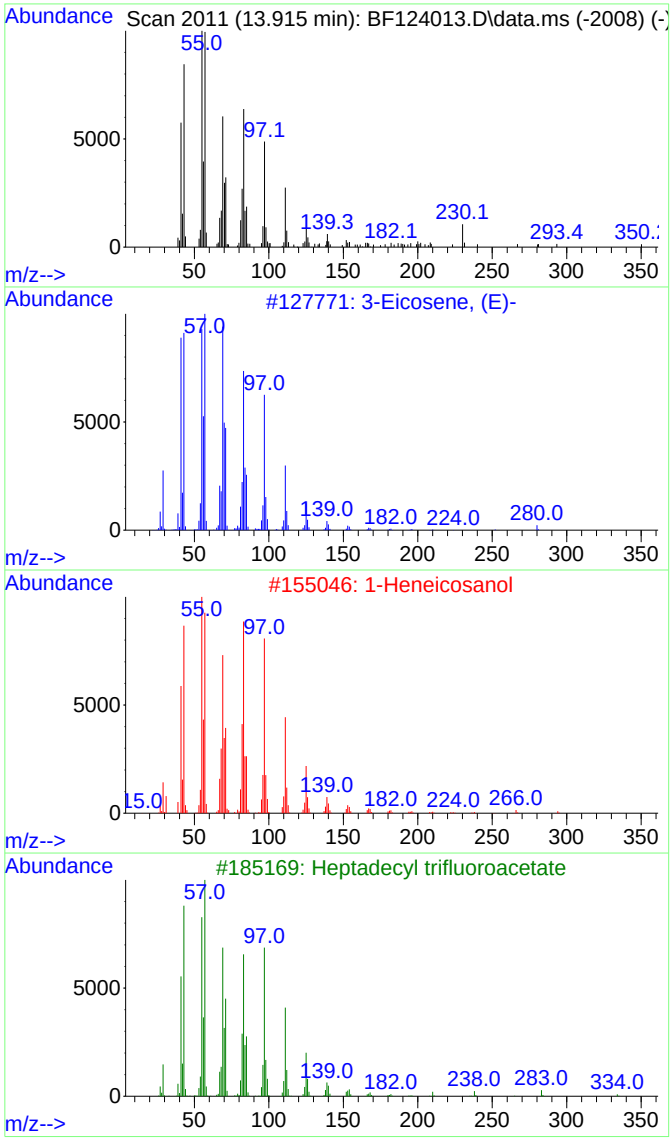
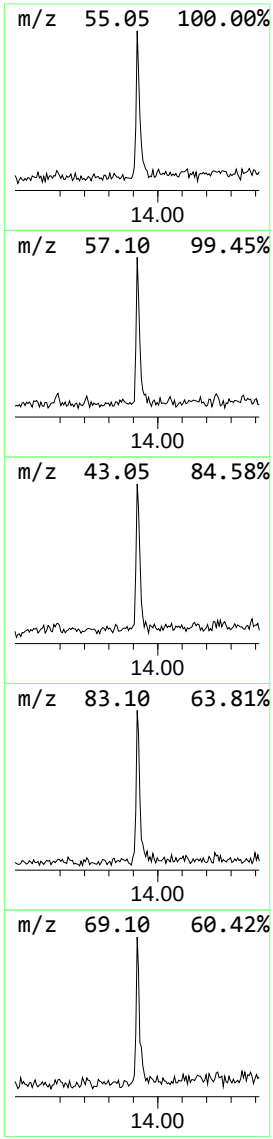
****

Peak Number 5 3-Eicosene, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.915	12.33 ng	277936	Chrysene-d12	14.074

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	98
2	1-Heneicosanol	312	C21H44O	015594-90-8	91
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
4	Cyclotetracosane	336	C24H48	000297-03-0	90
5	1-Octadecanol	270	C18H38O	000112-92-5	90





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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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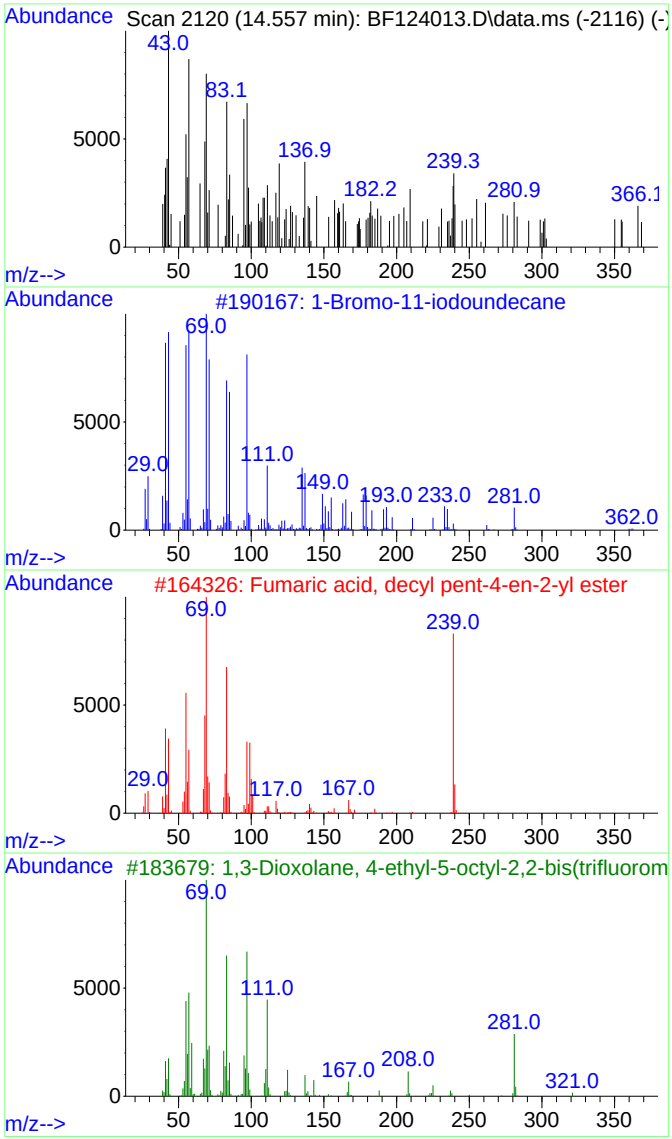
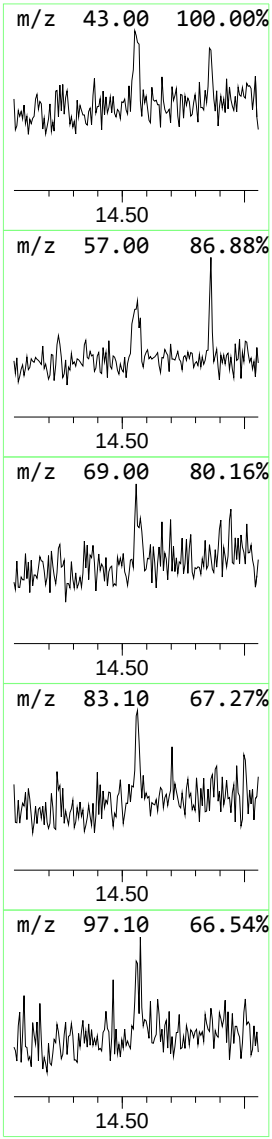
Peak Number 6 unknown14.55 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.557	2.41 ng	54319	Chrysene-d12	14.074

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Bromo-11-iodoundecane	360	C11H22BrI	139123-69-6	27
2	Fumaric acid, decyl pent-4-en-2-...	324	C19H32O4	1000348-92-9	16
3	1,3-Dioxolane, 4-ethyl-5-octyl-2...	350	C15H24F6O2	038274-73-6	16
4	4-Nonene, 5-butyl-	182	C13H26	007367-38-6	14
5	Hexadecanoic acid, 2-hydroxy-, m...	286	C17H34O3	016742-51-1	12





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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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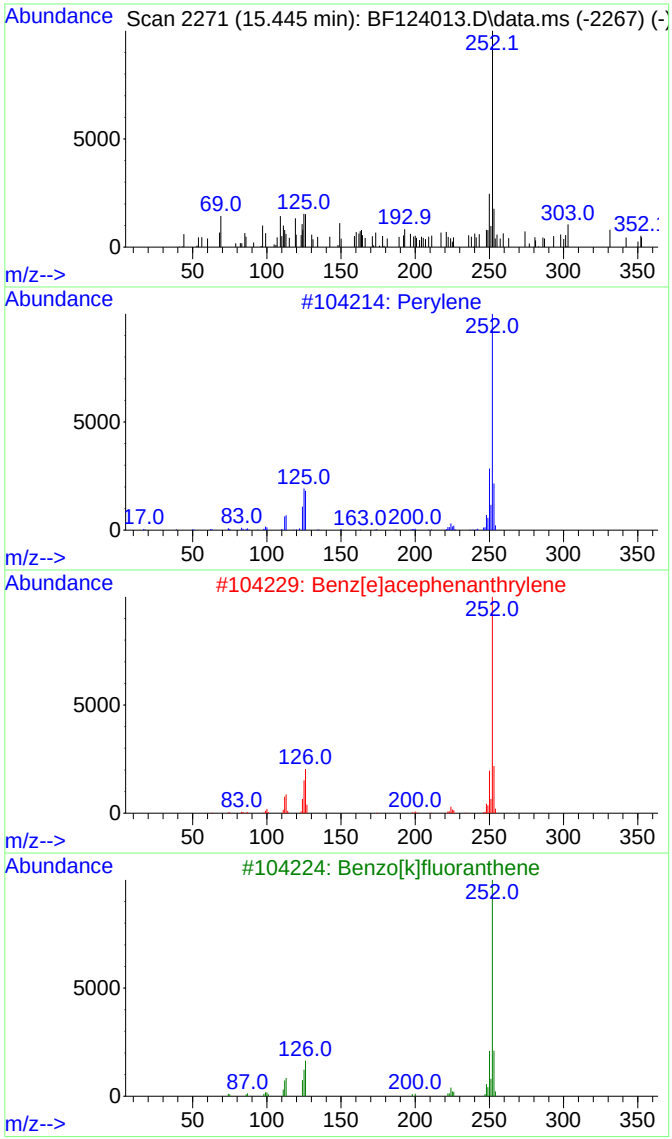
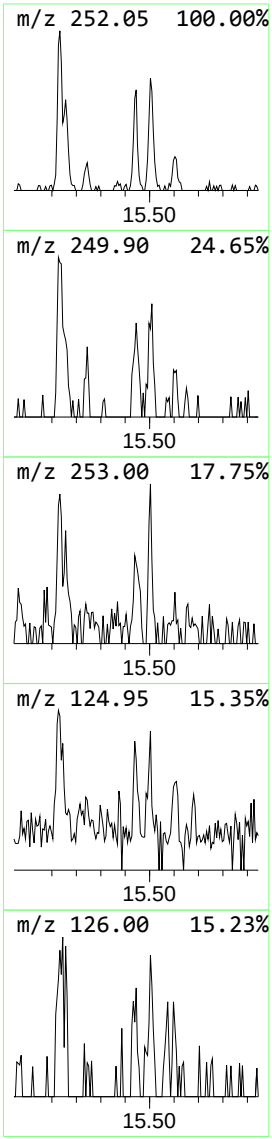
Peak Number 7 Perylene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.445	2.45 ng	34756	Perylene-d12	15.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	87
2	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	55
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	55
4	Benzo[e]pyrene	252	C20H12	000192-97-2	55
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	49





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Data File : BF124013.D
Acq On : 20 May 2021 17:18
Operator : JU/CG
Sample : M2462-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WATER-MAIN-BREAK-SOIL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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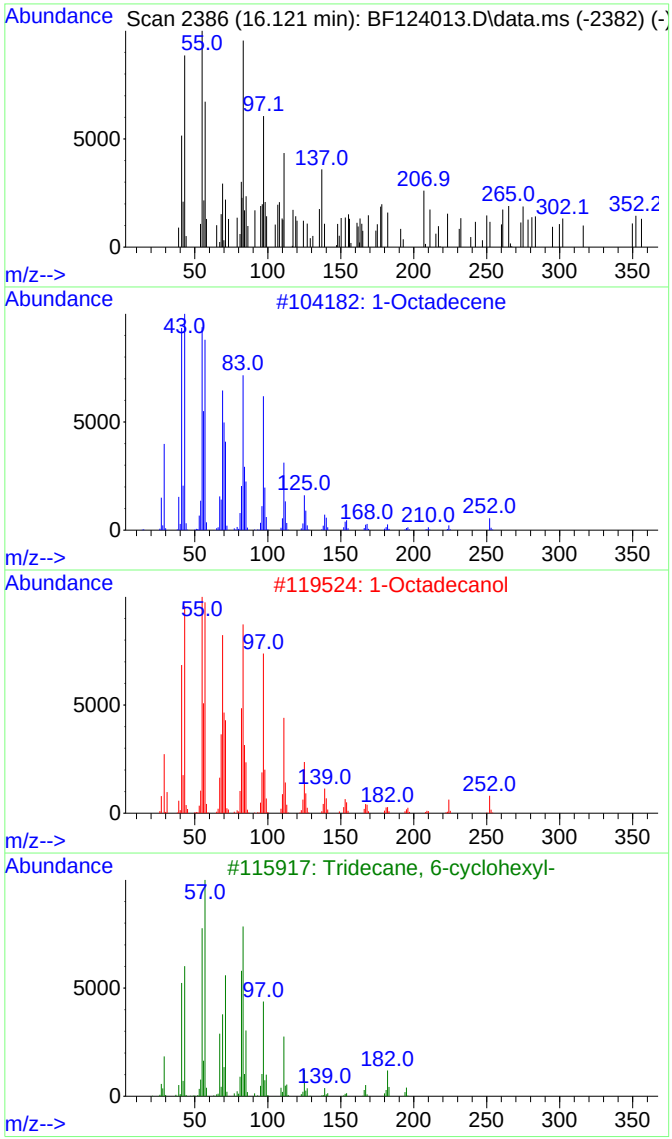
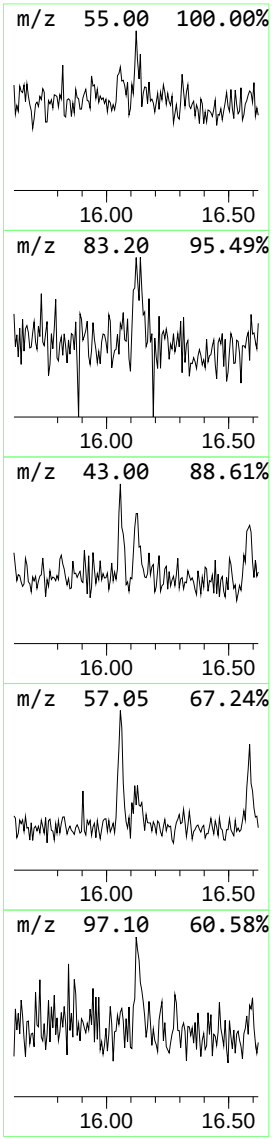
Peak Number 8 1-Octadecene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.121	4.53 ng	64362	Perylene-d12	15.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecene	252	C18H36	000112-88-9	62
2	1-Octadecanol	270	C18H38O	000112-92-5	58
3	Tridecane, 6-cyclohexyl-	266	C19H38	013151-91-2	53
4	Octacosyl acetate	452	C30H60O2	018206-97-8	43
5	E-15-Heptadecenal	252	C17H32O	1000130-97-9	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052021\
Data File : BF124013.D
Acq On : 20 May 2021 17:18
Operator : JU/CG
Sample : M2462-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WATER-MAIN-BREAK-SOIL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.146	43.8	ng	659104	1	6.904	300883	20.0
Propane, 1,1-di...	2.257	3.2	ng	47756	1	6.904	300883	20.0
2-Pentanone, 4-...	5.116	8.7	ng	130229	1	6.904	300883	20.0
Tridecanoic acid	11.951	3.6	ng	83903	4	11.433	470346	20.0
3-Eicosene, (E)-	13.915	12.3	ng	277936	5	14.074	451001	20.0
unknown14.55	14.557	2.4	ng	54319	5	14.074	451001	20.0
Perylene	15.445	2.5	ng	34756	6	15.574	284221	20.0
1-Octadecene	16.121	4.5	ng	64362	6	15.574	284221	20.0