LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101321\
Data File : BF125821.D
Acq On : 13 Oct 2021 12:07
Operator : JU/CG
Sample : M4117-15
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-5(0-0.5)

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-BF100721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125821.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	3	7	13	rVB	998294	1227384	24.57%	3.236%
2	5.069	498	507	513	rVB	49609	65283	1.31%	0.172%
3	5.463	569	574	577	rBV	4199444	3954562	79.16%	10.428%
4	6.469	739	745	748	rBV	3942752	3957934	79.23%	10.436%
5	6.840	805	808	812	rBV	1296699	1106133	22.14%	2.917%
6	7.404	899	904	907	rBV	2880790	2602976	52.10%	6.864%
7	8.028	1006	1010	1022	rBV	706257	698357	13.98%	1.841%
8	8.122	1022	1026	1029	rBV	1877488	1504591	30.12%	3.967%
9	9.198	1205	1209	1212	rBV	5747758	4995648	100.00%	13.173%
10	9.875	1320	1324	1328	rBV	2070808	1655876	33.15%	4.366%
11	10.663	1454	1458	1461	rBV	2931880	2586259	51.77%	6.820%
12	11.222	1548	1553	1557	rBV2	98363	92138	1.84%	0.243%
13	11.357	1572	1576	1579	rBV	1801122	1533796	30.70%	4.044%
14	11.380	1579	1580	1583	rVB	133924	82594	1.65%	0.218%
15	11.851	1656	1660	1663	rBV2	98371	154304	3.09%	0.407%
16	11.886	1663	1666	1672	rVB	521237	504587	10.10%	1.331%
17	12.410	1751	1755	1758	rBV	54737	63936	1.28%	0.169%
18	12.539	1774	1777	1779	rBV	55157	55340	1.11%	0.146%
19	12.569	1779	1782	1785	rBV	316400	254133	5.09%	0.670%
20	12.616	1785	1790	1792	rBV5	40664	58028	1.16%	0.153%
21	12.675	1794	1800	1806	rBV2	1037365	1319798	26.42%	3.480%
22	12.798	1817	1821	1824	rVB	287050	256300	5.13%	0.676%
23	12.886	1833	1836	1838	rBV	182178	159061	3.18%	0.419%
24	12.945	1842	1846	1849	rVV	4436166	3831210	76.69%	10.102%
25	13.227	1890	1894	1896	rBV3	59207	70060	1.40%	0.185%
26	13.516	1937	1943	1946	rBV	125680	132736	2.66%	0.350%
27	13.845	1995	1999	2008	rBV2	194356	316837	6.34%	0.835%
28	13.992	2016	2024	2027	rBV	1351424	1370278	27.43%	3.613%
29	14.016	2027	2028	2031	rVB	163373	96481	1.93%	0.254%
30	14.474	2102	2106	2113	rBV3	83279	205273	4.11%	0.541%
31	14.916	2178	2181	2187	rVB2	61117	74620	1.49%	0.197%
32	15.021	2195	2199	2207	rVB	162212	302033	6.05%	0.796%
33	15.104	2210	2213	2216	rBV	99289	122069	2.44%	0.322%
34	15.139	2216	2219	2225	rVB3	50202	85538	1.71%	0.226%
35	15.321	2247	2250	2256	rVB	98586	116951	2.34%	0.308%
36	15.386	2257	2261	2266	rVB	125213	151317	3.03%	0.399%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101321\
Data File : BF125821.D
Acq On : 13 Oct 2021 12:07
Operator : JU/CG
Sample : M4117-15
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-5(0-0.5)

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-BF100721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.451	2267	2272	2275	rVV	944801	1186123	23.74%	3.128%
38	15.480	2275	2277	2284	rVB3	81121	112257	2.25%	0.296%
39	15.686	2309	2312	2315	rVB3	53096	61734	1.24%	0.163%
40	15.921	2347	2352	2356	rBV	128559	179384	3.59%	0.473%
41	16.710	2482	2486	2495	rVB5	67812	142838	2.86%	0.377%
42	17.015	2533	2538	2544	rVB3	38874	72999	1.46%	0.192%
43	17.210	2566	2571	2575	rBV4	87761	158451	3.17%	0.418%
44	17.257	2575	2579	2586	rVB4	128676	246059	4.93%	0.649%

Sum of corrected areas: 37924266

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101321\
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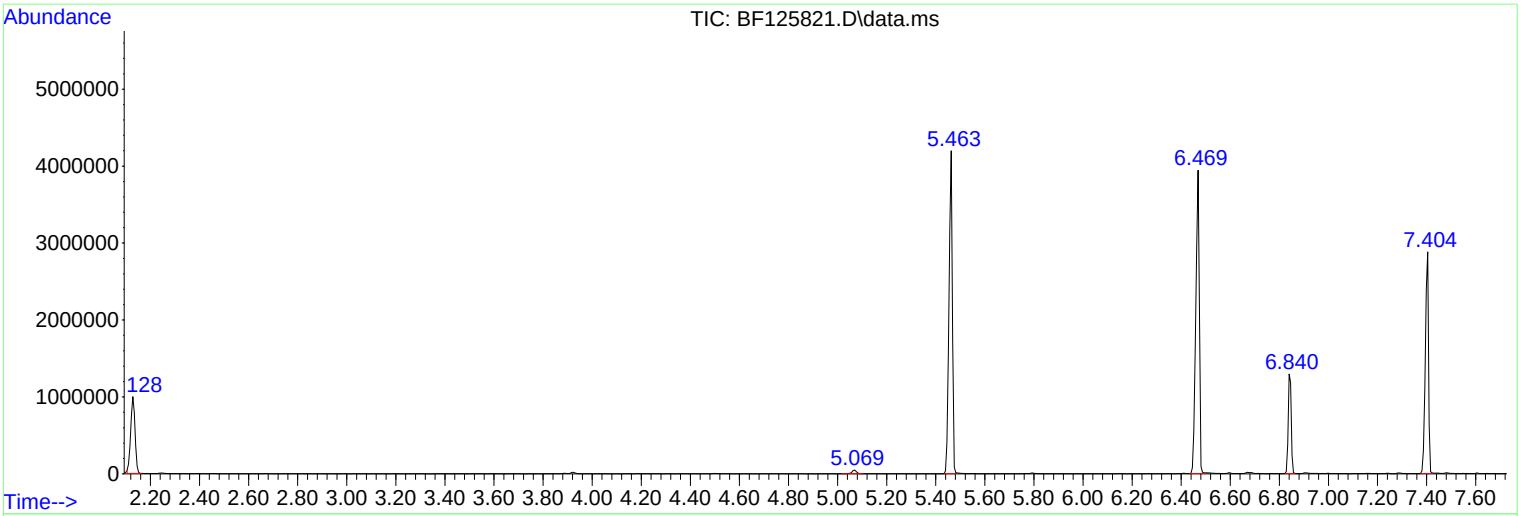
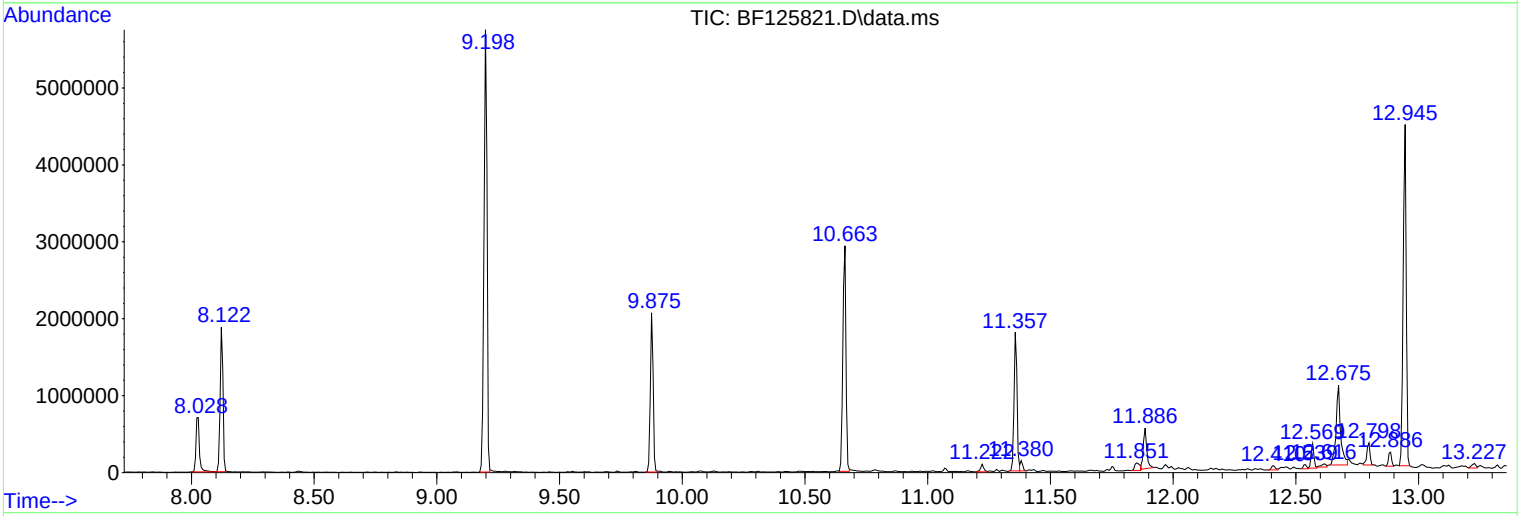
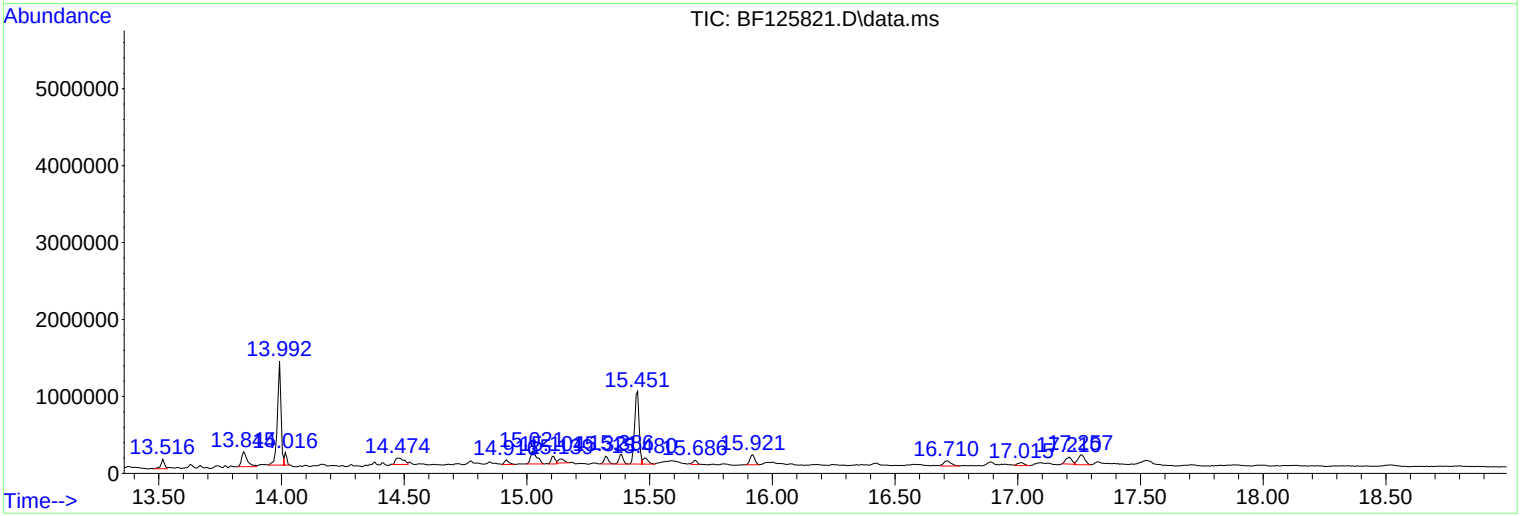
Instrument :
BNA_F
ClientSampleId :
SB-5(0-0.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.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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Data File : BF125821.D
Acq On : 13 Oct 2021 12:07
Operator : JU/CG
Sample : M4117-15
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-5(0-0.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

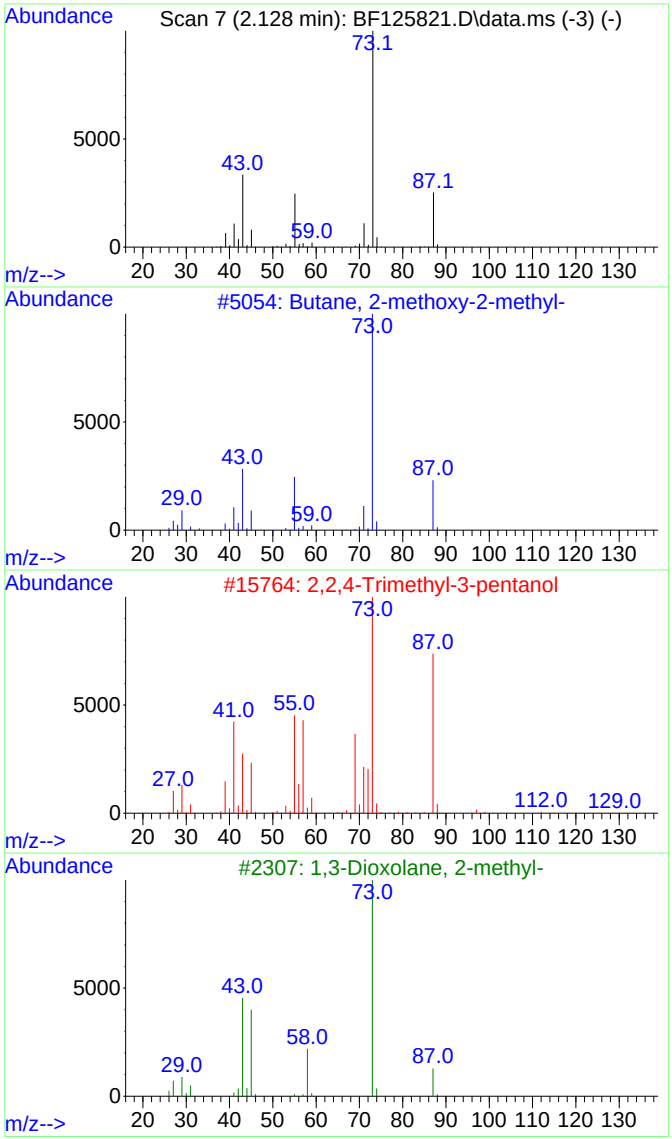
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

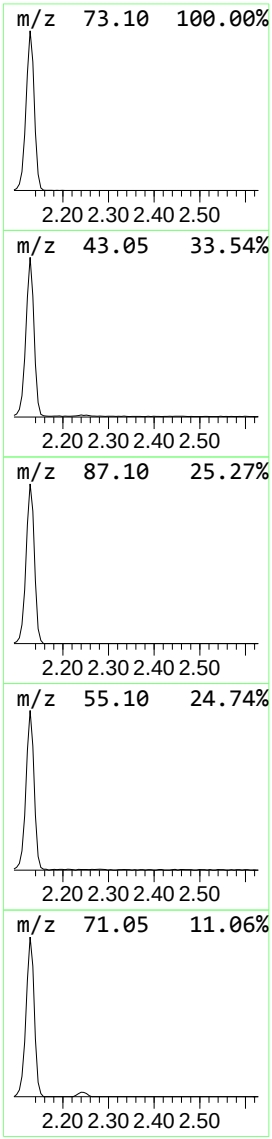
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.128	22.19 ng	1227380	1,4-Dichlorobenzene-d4	6.840

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





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Operator : JU/CG
Sample : M4117-15
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-5(0-0.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

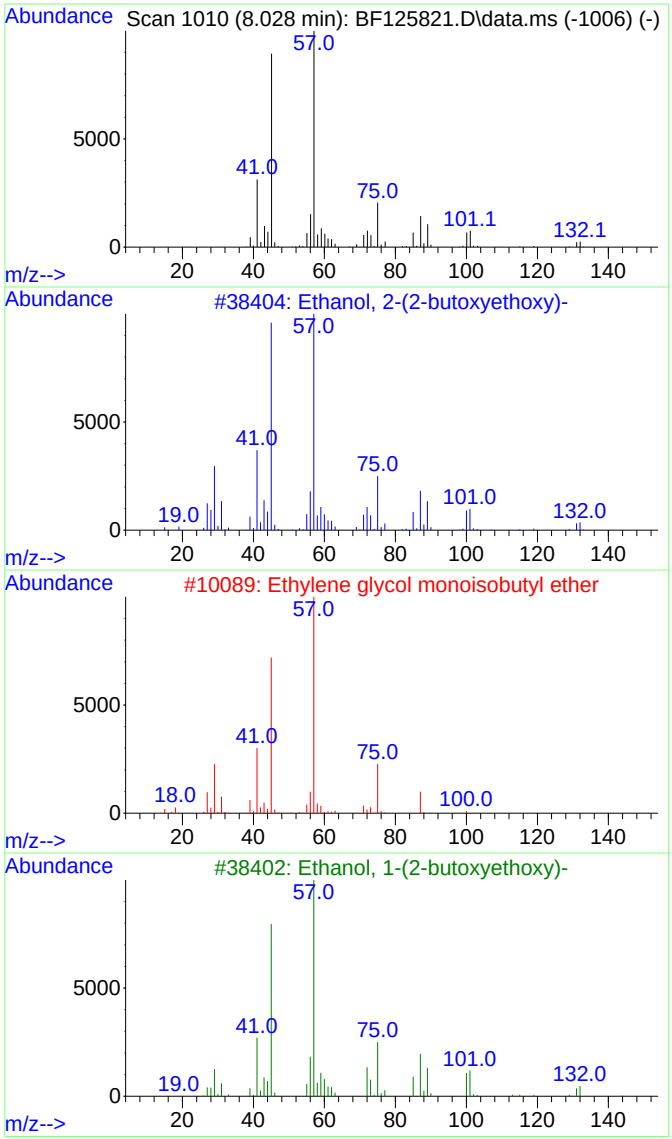
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

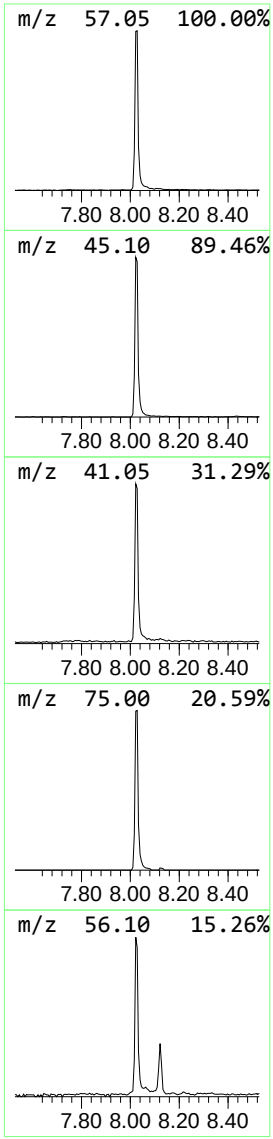
****

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.028	9.28 ng	698357	Naphthalene-d8	8.122

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	91
2	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
3	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	58
4	Di-sec-Butyl ether	130	C8H18O	006863-58-7	50
5	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101321\
Data File : BF125821.D
Acq On : 13 Oct 2021 12:07
Operator : JU/CG
Sample : M4117-15
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-5(0-0.5)

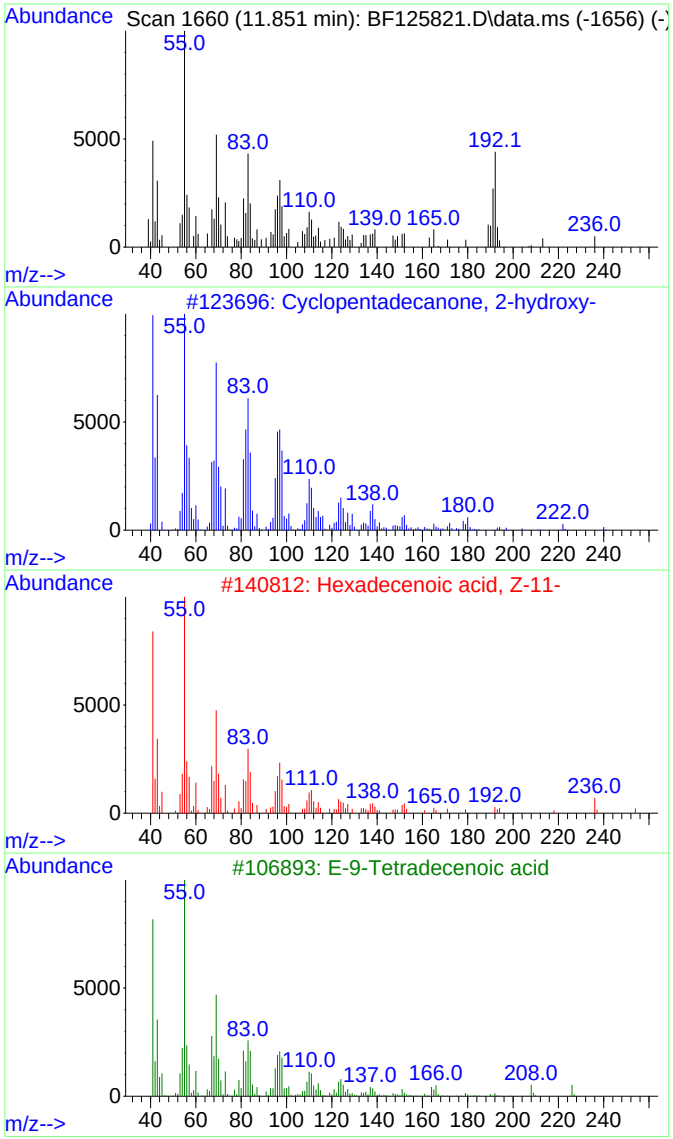
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

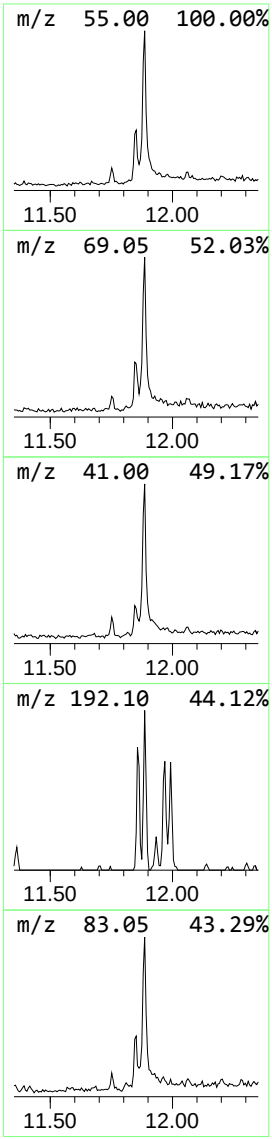
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclopentadecanone, 2-hydroxy- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.851	2.01 ng	154304	Phenanthrene-d10	11.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecanone, 2-hydroxy-	240	C15H28O2	004727-18-8	50
2	Hexadecenoic acid, Z-11-	254	C16H30O2	002416-20-8	46
3	E-9-Tetradecenoic acid	226	C14H26O2	050286-30-1	35
4	Palmitoleic acid	254	C16H30O2	000373-49-9	30
5	9-Oxabicyclo[6.1.0]nonane, cis-	126	C8H14O	004925-71-7	30





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Operator : JU/CG
Sample : M4117-15
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-5(0-0.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

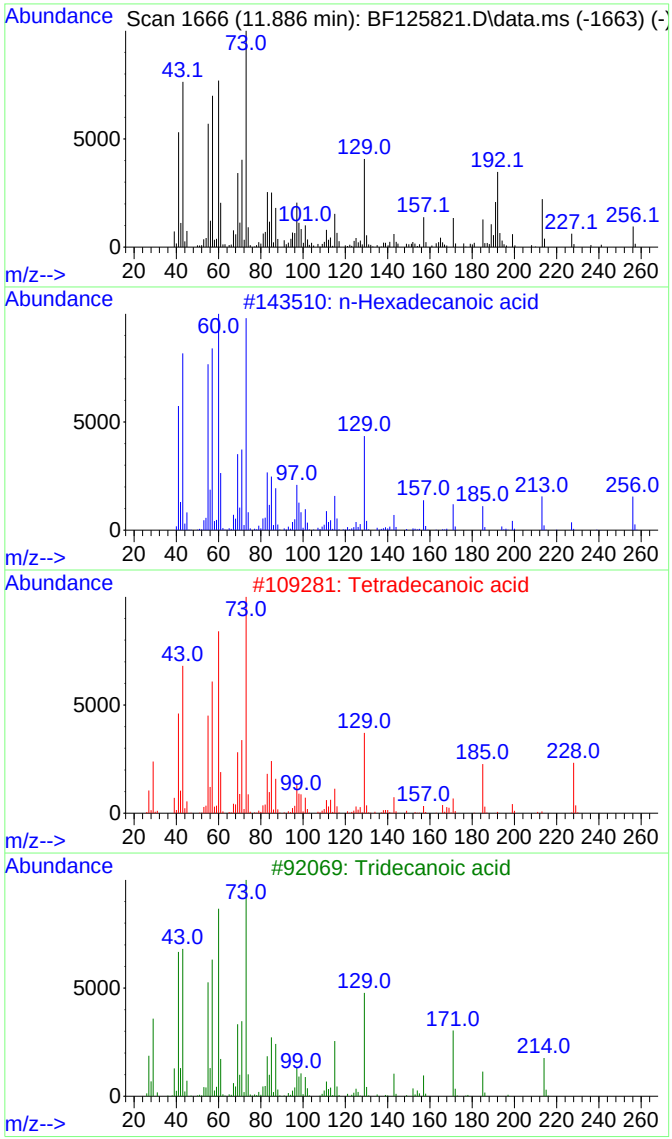
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

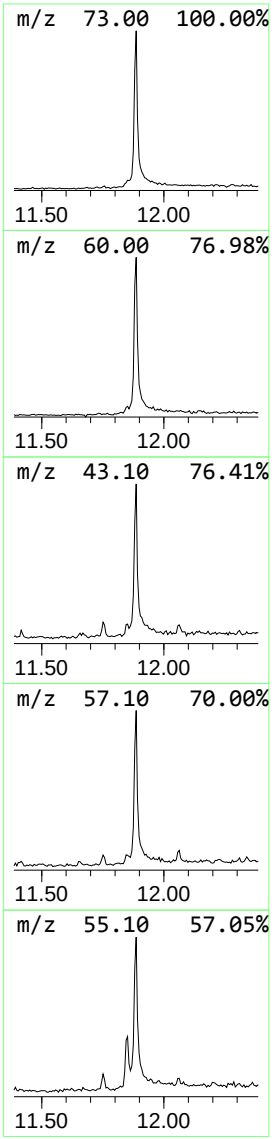
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.886	6.58 ng	504587	Phenanthrene-d10	11.357

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	89
3	Tridecanoic acid	214	C13H26O2	000638-53-9	78
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	70
5	n-Decanoic acid	172	C10H20O2	000334-48-5	58





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Data File : BF125821.D
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Operator : JU/CG
Sample : M4117-15
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-5(0-0.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

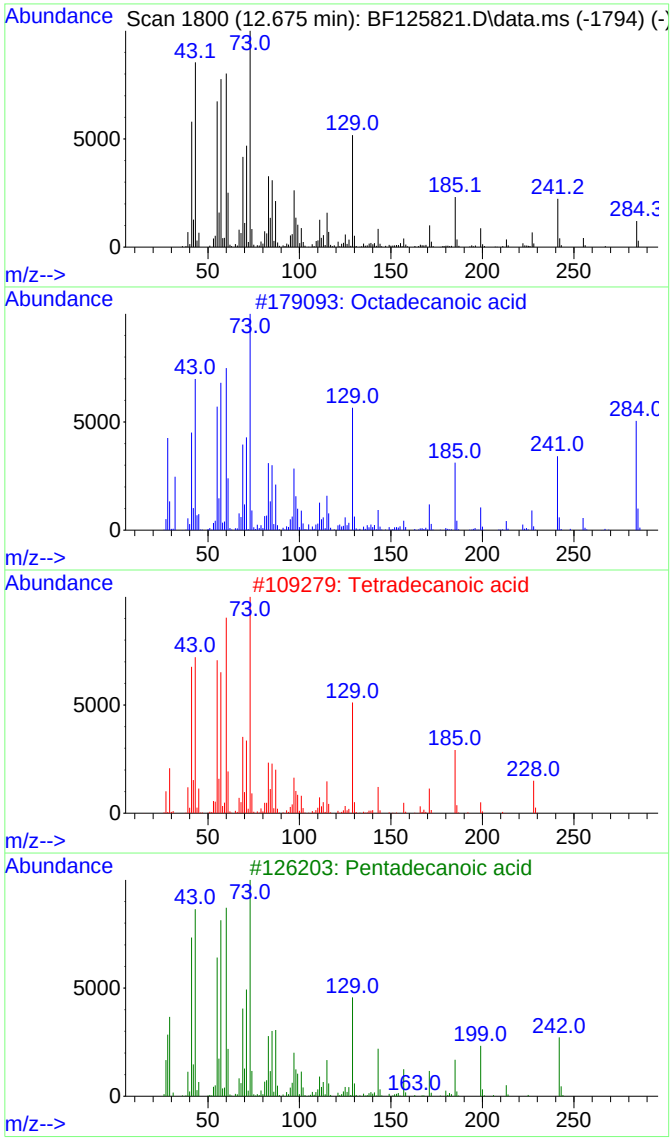
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

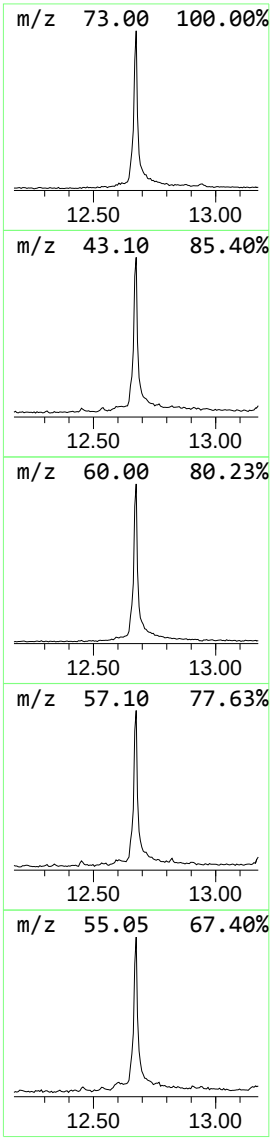
****

Peak Number 5 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.675	17.21 ng	1319800	Phenanthrene-d10	11.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	53





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ClientSampleId : SB-5(0-0.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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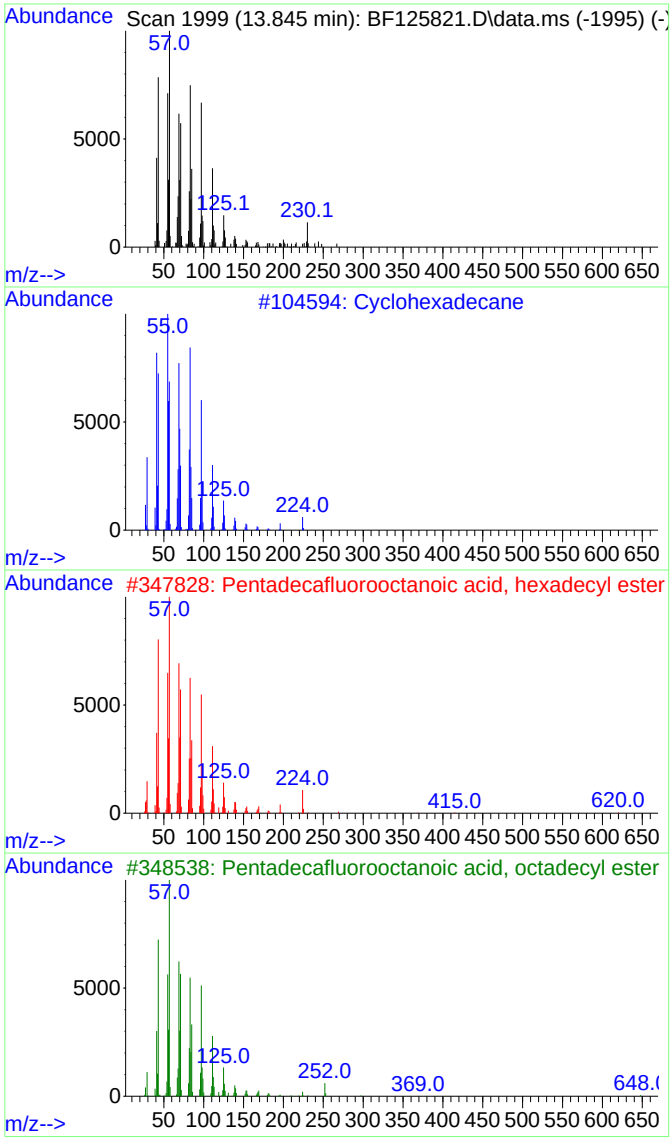
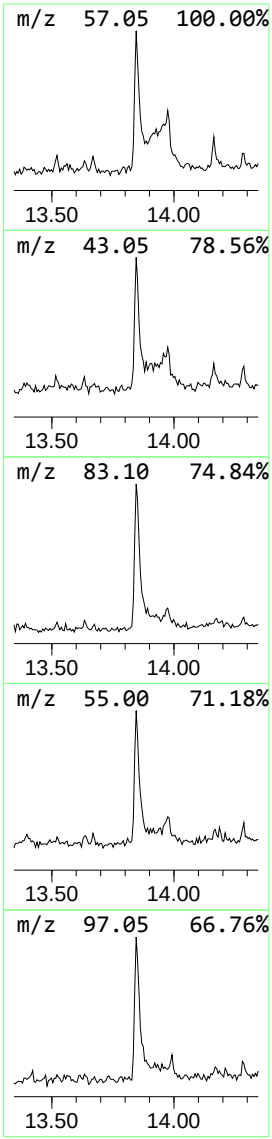
****

Peak Number 7 Cyclohexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.845	4.62 ng	316837	Chrysene-d12	13.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	95
2	Pentadecafluorooctanoic acid, he...	638	C24H33F15O2	1000406-04-6	94
3	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
4	1-Heneicosanol	312	C21H44O	015594-90-8	93
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93





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Sample : M4117-15
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-5(0-0.5)

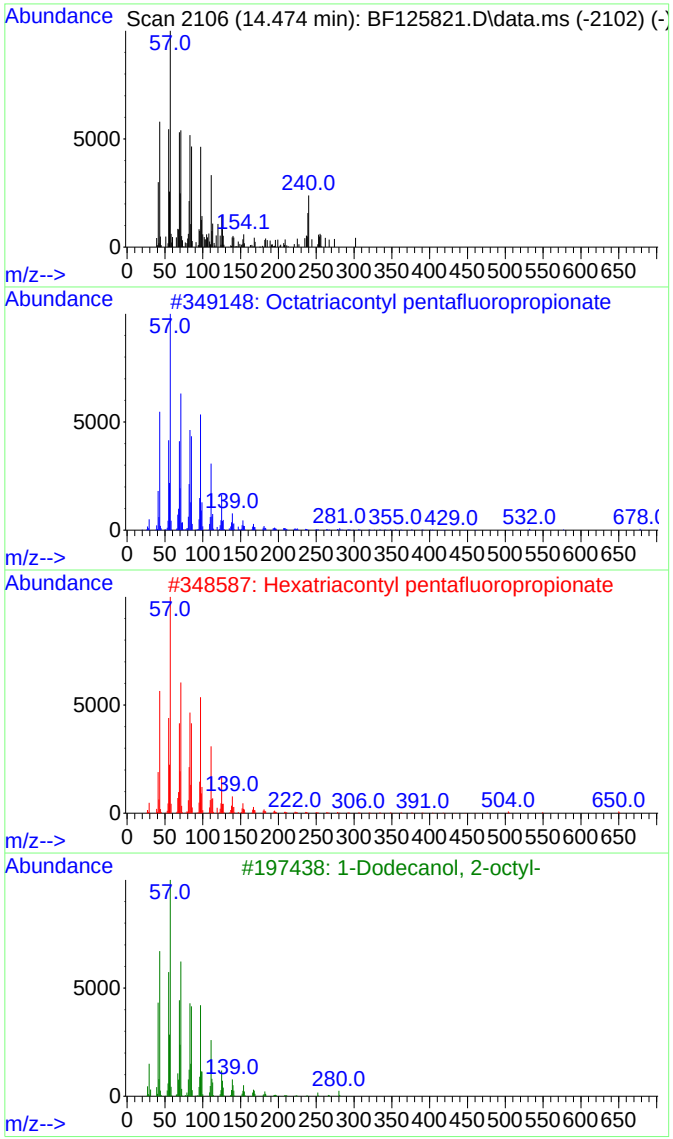
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

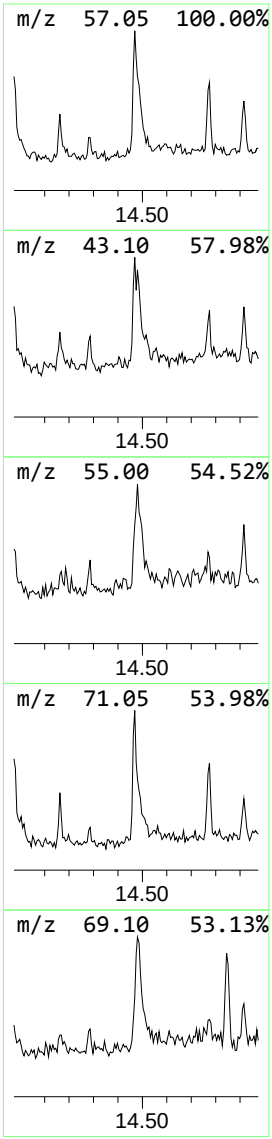
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Octatriacontyl pentafluorop... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.474	3.00 ng	205273	Chrysene-d12	13.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	81
2	Hexatriacontyl pentafluoropropio...	669	C39H73F5O2	1000351-89-0	74
3	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	74
4	Tetratriacontyl pentafluoropropi...	641	C37H69F5O2	1000351-81-5	74
5	Octacosyl heptafluorobutyrate	606	C32H57F7O2	1010351-83-6	74





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Data File : BF125821.D
Acq On : 13 Oct 2021 12:07
Operator : JU/CG
Sample : M4117-15
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-5(0-0.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

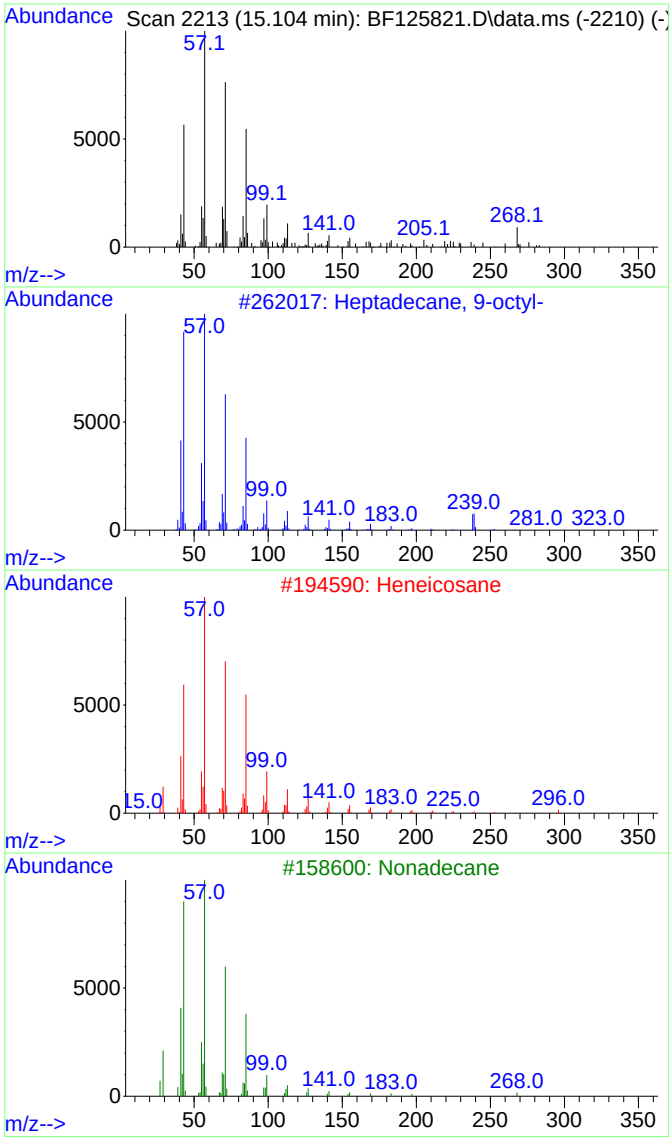
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

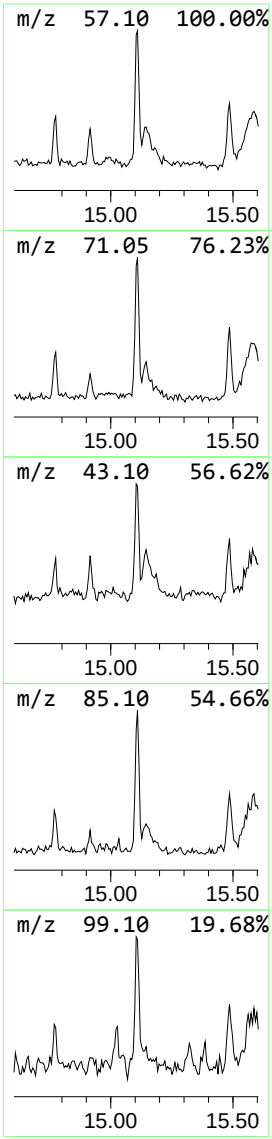
****

Peak Number 9 Heptadecane, 9-octyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.104	2.06 ng	122069	Perylene-d12	15.451

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
2	Heneicosane	296	C21H44	000629-94-7	87
3	Nonadecane	268	C19H40	000629-92-5	87
4	Hexacosane	366	C26H54	000630-01-3	87
5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	86





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Data File : BF125821.D
Acq On : 13 Oct 2021 12:07
Operator : JU/CG
Sample : M4117-15
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-5(0-0.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.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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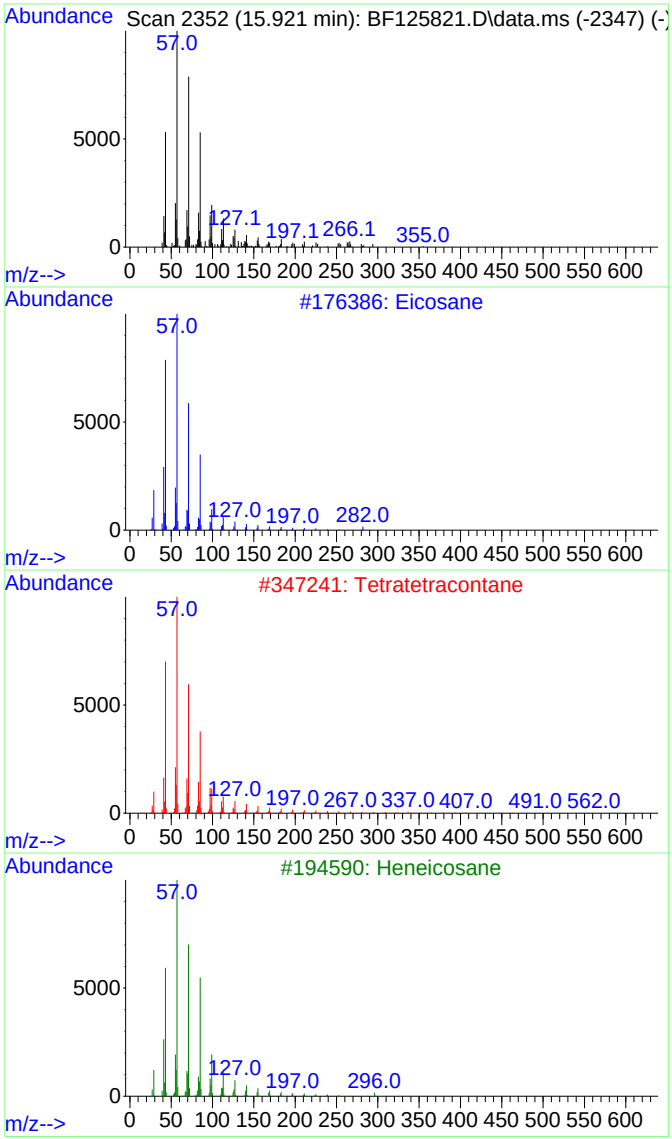
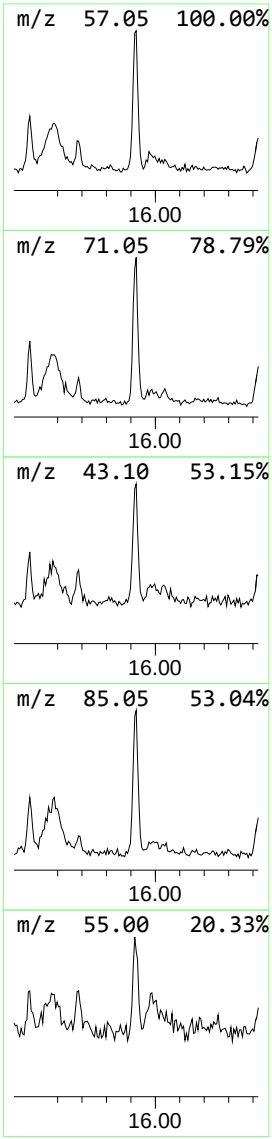
Peak Number 10 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.921	3.02 ng	179384	Perylene-d12	15.451

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Tetratetracontane	619	C44H90	007098-22-8	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Triacontane	422	C30H62	000638-68-6	91





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Acq On : 13 Oct 2021 12:07
Operator : JU/CG
Sample : M4117-15
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-5(0-0.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.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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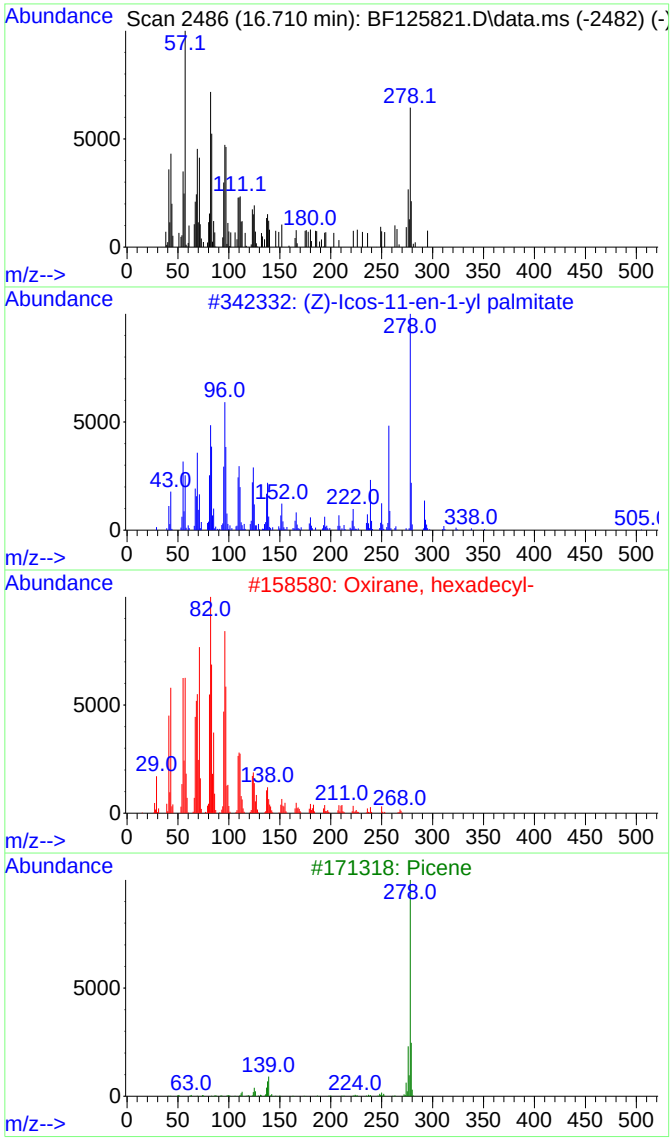
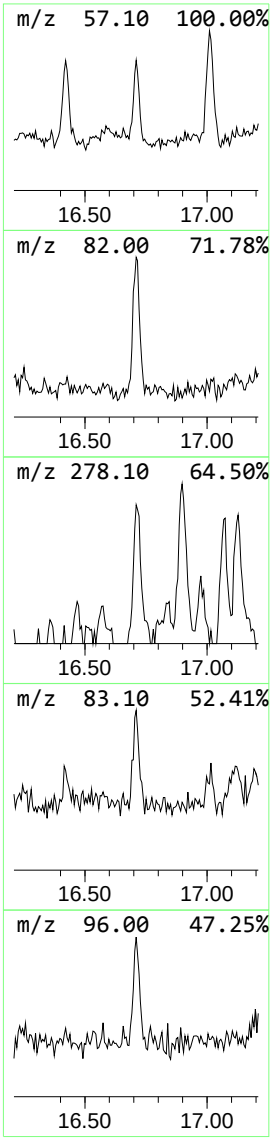
Peak Number 11 unknown16.709 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.709	2.41 ng	142838	Perylene-d12	15.451

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(Z)-Icos-11-en-1-yl palmitate	535	C36H70O2	174305-42-1	38
2	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	30
3	Picene	278	C22H14	000213-46-7	25
4	Disulfide, bis(2-methoxyphenyl)	278	C14H14O2S2	013920-94-0	25
5	Benzo[b]triphenylene	278	C22H14	000215-58-7	22





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Data File : BF125821.D
Acq On : 13 Oct 2021 12:07
Operator : JU/CG
Sample : M4117-15
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-5(0-0.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.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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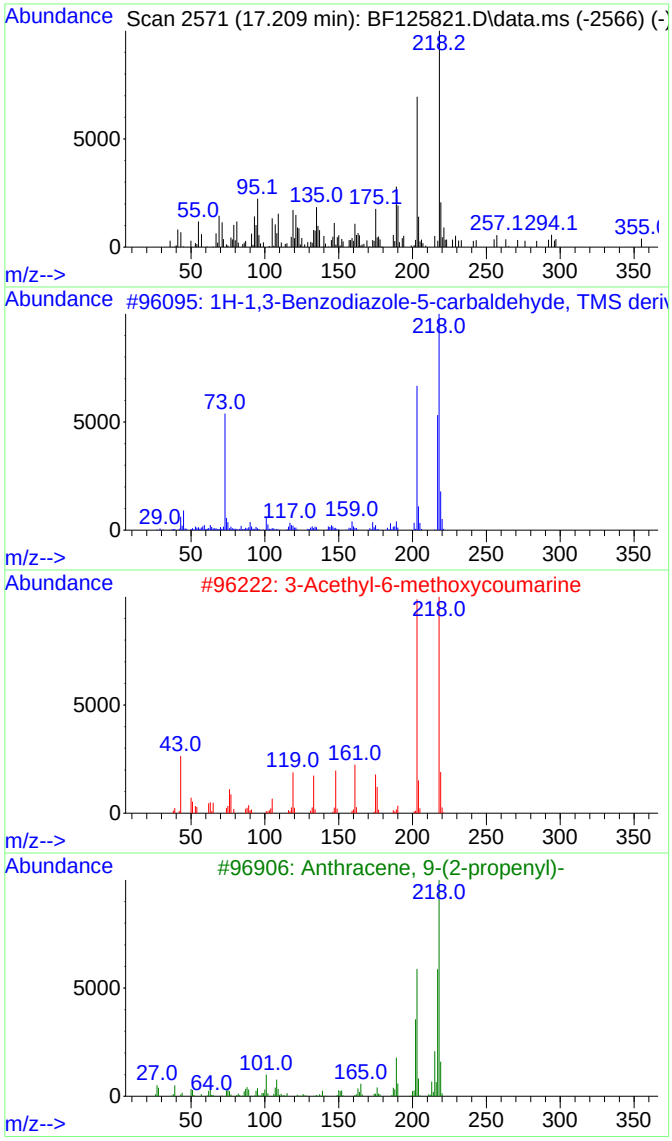
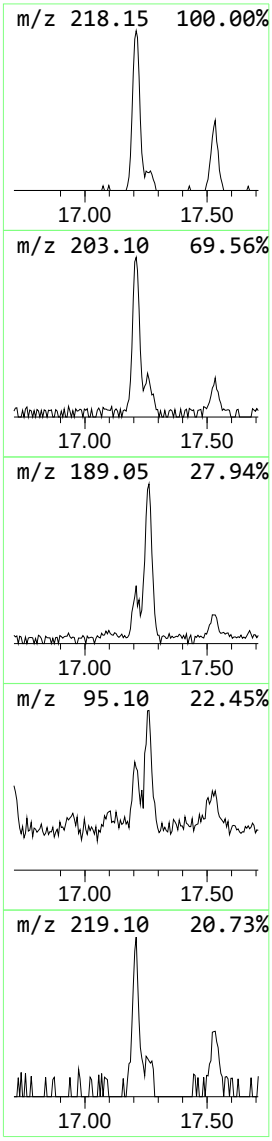
Peak Number 12 1H-1,3-Benzodiazole-5-carba... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.209	2.67 ng	158451	Perylene-d12	15.451

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-1,3-Benzodiazole-5-carbaldehy...	218	C11H14N2OSi	1000478-28-4	64
2	3-Acethyl-6-methoxycoumarine	218	C12H10O4	013252-80-7	52
3	Anthracene, 9-(2-propenyl)-	218	C17H14	023707-65-5	52
4	.alpha.-Amyrin, TMS derivative	498	C33H58OSi	1000374-76-6	49
5	Benzo[b]naphtho[2,3-d]furan	218	C16H10O	000243-42-5	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101321\
Data File : BF125821.D
Acq On : 13 Oct 2021 12:07
Operator : JU/CG
Sample : M4117-15
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-5(0-0.5)

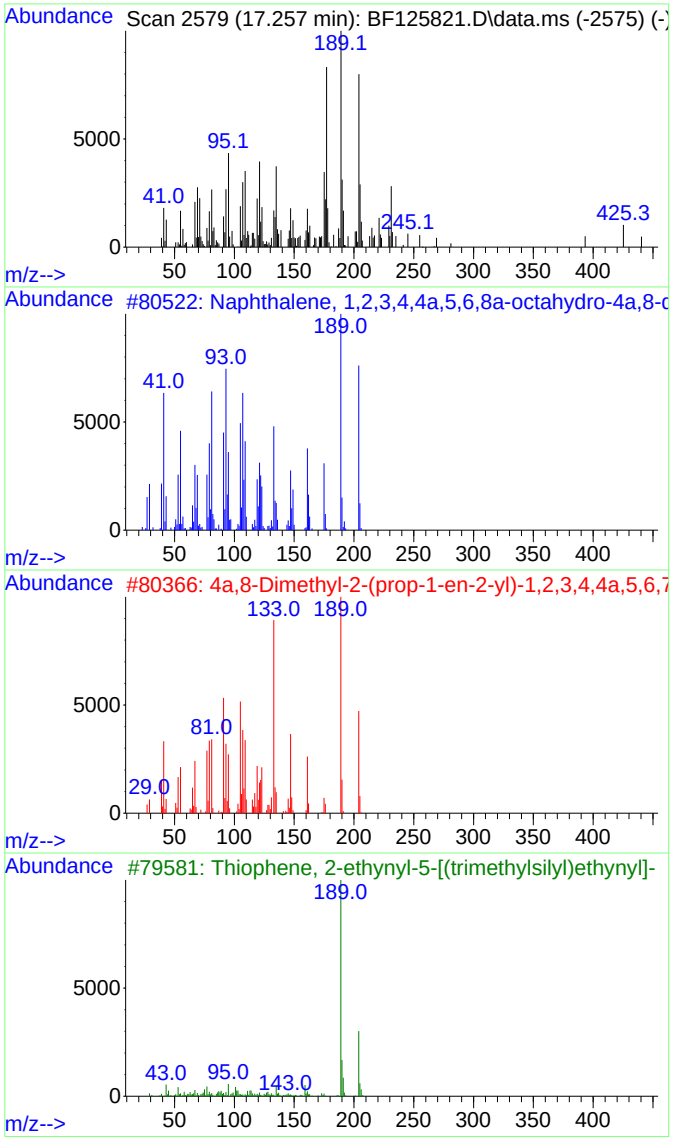
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

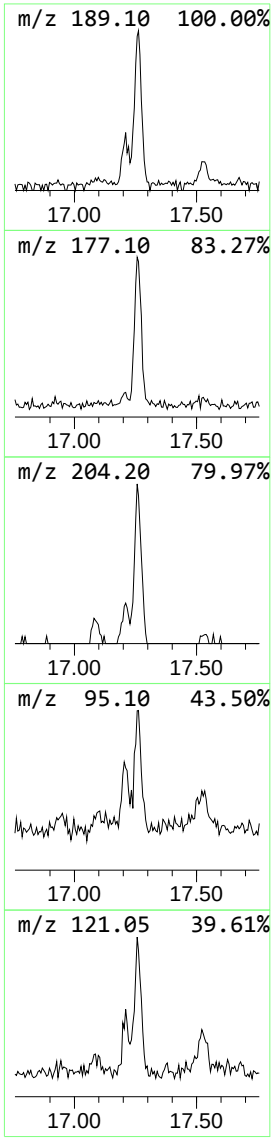
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 Naphthalene, 1,2,3,4,4a,5,6... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.257	4.15 ng	246059	Perylene-d12	15.451

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4,4a,5,6,8a-o...	204	C15H24	000473-13-2	60
2	4a,8-Dimethyl-2-(prop-1-en-2-yl)...	204	C15H24	103827-22-1	55
3	Thiophene, 2-ethynyl-5-[(trimeth...	204	C11H12SSi	182323-29-1	49
4	1H-Cyclopropa[a]naphthalene, 1a,...	204	C15H24	000489-29-2	49
5	2-Naphthalenemethanol, 1,2,3,4,4...	222	C15H26O	001209-71-8	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101321\
Data File : BF125821.D
Acq On : 13 Oct 2021 12:07
Operator : JU/CG
Sample : M4117-15
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-5(0-0.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.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...	2.128	22.2	ng	1227380	1	6.840	1106130	20.0
Ethanol, 2-(2-b...	8.028	9.3	ng	698357	2	8.122	1504590	20.0
Cyclopentadecan...	11.851	2.0	ng	154304	4	11.357	1533800	20.0
n-Hexadecanoic ...	11.886	6.6	ng	504587	4	11.357	1533800	20.0
Octadecanoic acid	12.675	17.2	ng	1319800	4	11.357	1533800	20.0
Cyclohexadecane	13.845	4.6	ng	316837	5	13.992	1370280	20.0
Octatriacontyl ...	14.474	3.0	ng	205273	5	13.992	1370280	20.0
Heptadecane, 9-...	15.104	2.1	ng	122069	6	15.451	1186120	20.0
Eicosane	15.921	3.0	ng	179384	6	15.451	1186120	20.0
unknown16.709	16.709	2.4	ng	142838	6	15.451	1186120	20.0
1H-1,3-Benzodia...	17.209	2.7	ng	158451	6	15.451	1186120	20.0
Naphthalene, 1,...	17.257	4.2	ng	246059	6	15.451	1186120	20.0