LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050423\
Data File : BF133247.D
Acq On : 04 May 2023 23:41
Operator : CG\JU
Sample : 02588-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ZONE-C-0-3-05012023

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-BF042123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133247.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.710	270	276	281	rVB	121906	177261	4.18%	0.477%
2	4.916	477	481	487	rBV	85207	113015	2.66%	0.304%
3	5.334	548	552	556	rBV	3601636	3698407	87.14%	9.957%
4	5.734	614	620	625	rBV2	37480	64995	1.53%	0.175%
5	5.975	658	661	663	rBV	85980	74944	1.77%	0.202%
6	6.034	668	671	673	rBV	75688	65711	1.55%	0.177%
7	6.163	688	693	696	rBV2	72861	88943	2.10%	0.239%
8	6.257	706	709	717	rBV	202055	236837	5.58%	0.638%
9	6.363	722	727	730	rVV	3833318	3963400	93.38%	10.670%
10	6.398	730	733	735	rVB	66737	60495	1.43%	0.163%
11	6.469	741	745	749	rBV4	58679	98973	2.33%	0.266%
12	6.569	757	762	764	rBV3	92858	102570	2.42%	0.276%
13	6.669	774	779	782	rBV5	34459	57643	1.36%	0.155%
14	6.722	785	788	791	rVV	1341460	1182876	27.87%	3.185%
15	6.745	791	792	796	rVB	168538	108558	2.56%	0.292%
16	6.786	796	799	802	rBV3	77279	82873	1.95%	0.223%
17	6.875	812	814	818	rVB2	83044	76793	1.81%	0.207%
18	6.998	832	835	840	rVB3	106139	131600	3.10%	0.354%
19	7.075	845	848	853	rBV4	53853	66182	1.56%	0.178%
20	7.122	853	856	858	rBV	129626	111963	2.64%	0.301%
21	7.251	874	878	880	rBV	64048	80287	1.89%	0.216%
22	7.292	880	885	887	rVV	2582403	2607579	61.44%	7.020%
23	7.333	889	892	895	rVV	88559	83818	1.97%	0.226%
24	7.375	895	899	903	rVB4	71449	99704	2.35%	0.268%
25	7.504	915	921	922	rBV4	34233	58561	1.38%	0.158%
26	7.533	924	926	930	rVB2	57902	52640	1.24%	0.142%
27	7.651	939	946	951	rVB6	49912	94130	2.22%	0.253%
28	8.010	1003	1007	1010	rBV	1980316	1547888	36.47%	4.167%
29	9.086	1186	1190	1193	rBV	5230942	4244154	100.00%	11.426%
30	9.757	1301	1304	1308	rBV	2020574	1667704	39.29%	4.490%
31	10.304	1394	1397	1399	rBV	66001	50240	1.18%	0.135%
32	10.469	1421	1425	1429	rBV	357005	308558	7.27%	0.831%
33	10.545	1434	1438	1442	rBV	2729210	2533357	59.69%	6.820%
34	11.239	1552	1556	1558	rBV	1984812	1580002	37.23%	4.254%
35	11.263	1558	1560	1563	rVV	577401	431395	10.16%	1.161%
36	11.316	1563	1569	1572	rVB	116060	126276	2.98%	0.340%

LSC Area Percent Report

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Misc :
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Instrument :
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ClientSampleId :
ZONE-C-0-3-05012023

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-BF042123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	11.469	1590	1595	1598	rBV	58159	62664	1.48%	0.169%
38	11.739	1638	1641	1644	rBV	69956	61311	1.44%	0.165%
39	11.780	1644	1648	1652	rBV2	440549	478224	11.27%	1.287%
40	11.851	1657	1660	1663	rBV	101860	101468	2.39%	0.273%
41	12.451	1758	1762	1765	rBV	670954	619005	14.58%	1.666%
42	12.498	1765	1770	1776	rVB7	36460	62947	1.48%	0.169%
43	12.563	1778	1781	1786	rBV3	68701	76726	1.81%	0.207%
44	12.674	1794	1800	1803	rBV	593666	563102	13.27%	1.516%
45	12.827	1822	1826	1829	rBV	3855731	3256586	76.73%	8.767%
46	13.004	1854	1856	1859	rVB	88694	85993	2.03%	0.232%
47	13.068	1864	1867	1871	rBV2	114288	112504	2.65%	0.303%
48	13.110	1871	1874	1876	rBV	58271	57613	1.36%	0.155%
49	13.310	1905	1908	1917	rVB	133484	145148	3.42%	0.391%
50	13.410	1922	1925	1927	rBV	67322	55625	1.31%	0.150%
51	13.621	1958	1961	1963	rBV2	53178	60908	1.44%	0.164%
52	13.739	1977	1981	1995	rVB2	252387	462691	10.90%	1.246%
53	13.874	1999	2004	2006	rBV2	1265513	1330202	31.34%	3.581%
54	13.898	2006	2008	2011	rVB	272486	209880	4.95%	0.565%
55	14.357	2083	2086	2088	rBV2	162328	144548	3.41%	0.389%
56	14.657	2135	2137	2143	rVB2	83778	82215	1.94%	0.221%
57	14.792	2158	2160	2164	rVB3	59906	57198	1.35%	0.154%
58	14.886	2172	2176	2185	rVB	279057	503017	11.85%	1.354%
59	14.980	2188	2192	2196	rVB2	164735	210113	4.95%	0.566%
60	15.168	2221	2224	2230	rVB	161298	195293	4.60%	0.526%
61	15.227	2231	2234	2240	rVB	207030	215010	5.07%	0.579%
62	15.292	2240	2245	2248	rBV	892870	1057500	24.92%	2.847%
63	15.521	2281	2284	2291	rVB2	146791	202417	4.77%	0.545%
64	15.745	2318	2322	2327	rBV2	143212	211571	4.98%	0.570%
65	16.492	2445	2449	2460	rVB3	110806	208698	4.92%	0.562%
66	16.656	2473	2477	2483	rVB2	73555	123540	2.91%	0.333%

Sum of corrected areas: 37144049

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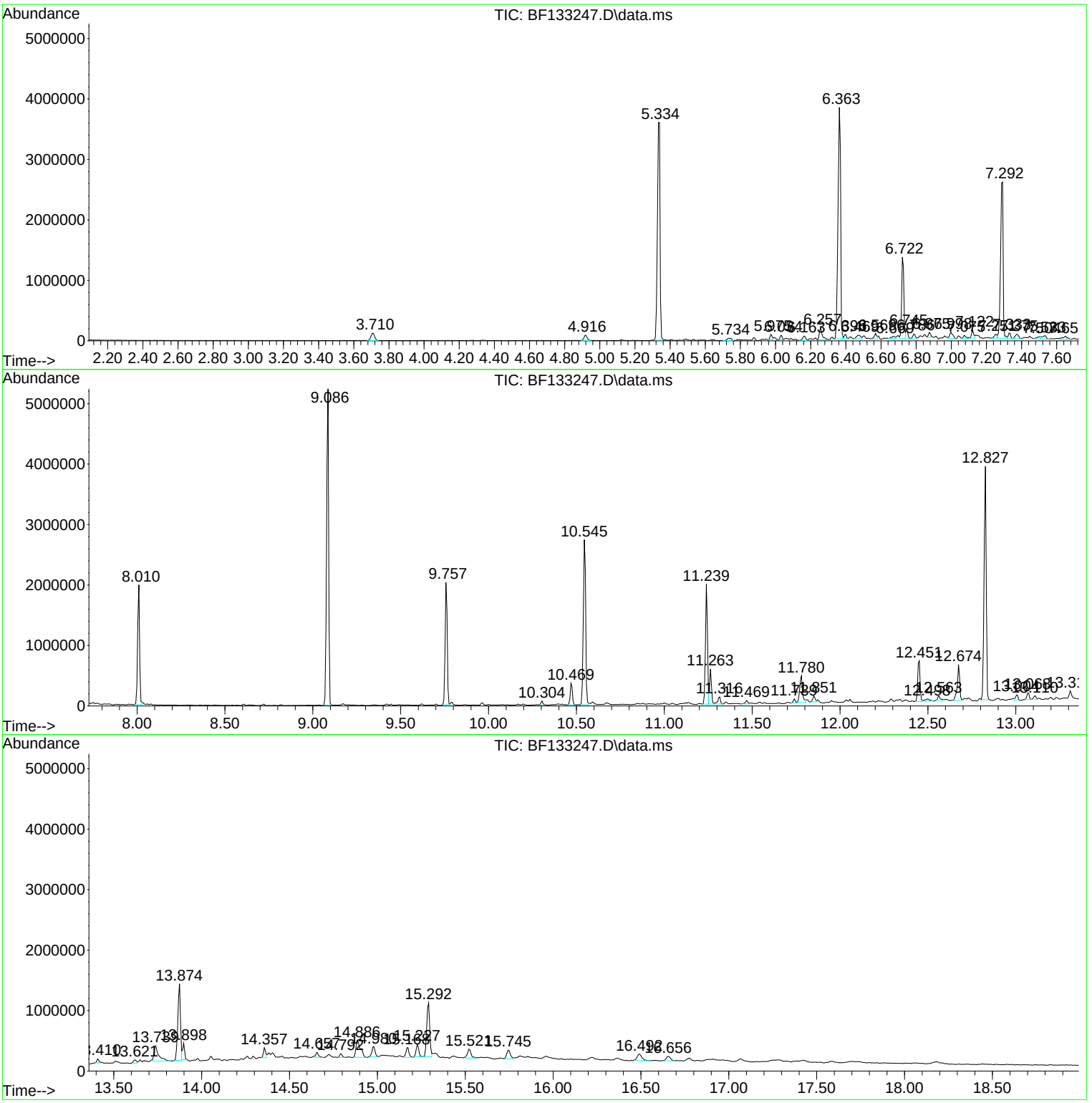
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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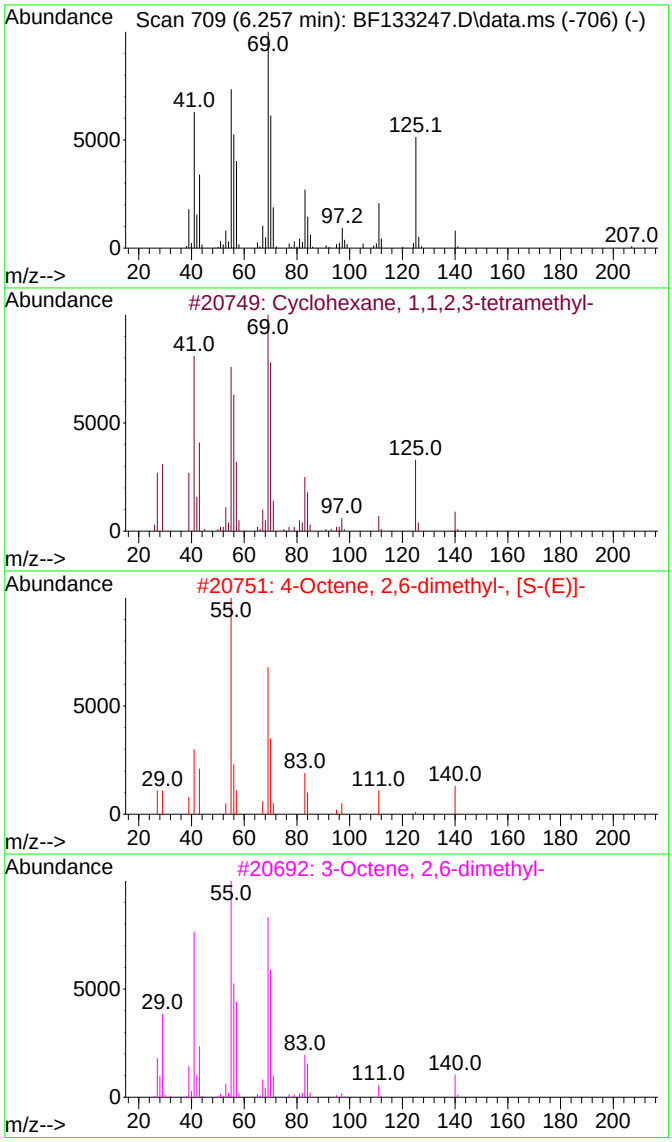
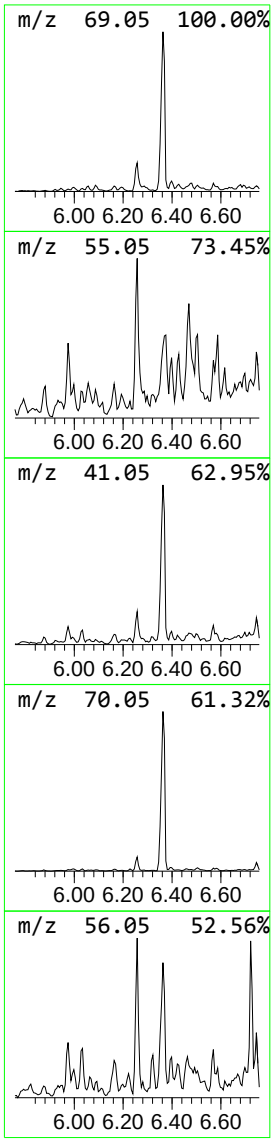
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Cyclohexane, 1,1,2,3-tetram... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.257	4.00 ng	236837	1,4-Dichlorobenzene-d4	6.722

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,1,2,3-tetramethyl-	140	C10H20	006783-92-2	93
2	4-Octene, 2,6-dimethyl-, [S-(E)]-	140	C10H20	062960-76-3	68
3	3-Octene, 2,6-dimethyl-	140	C10H20	006874-28-8	50
4	2-Octene, 2,6-dimethyl-	140	C10H20	004057-42-5	49
5	1-Hexene, 3,3-dimethyl-	112	C8H16	003404-77-1	46





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Misc :
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Instrument :
BNA_F
ClientSampleId :
ZONE-C-0-3-05012023

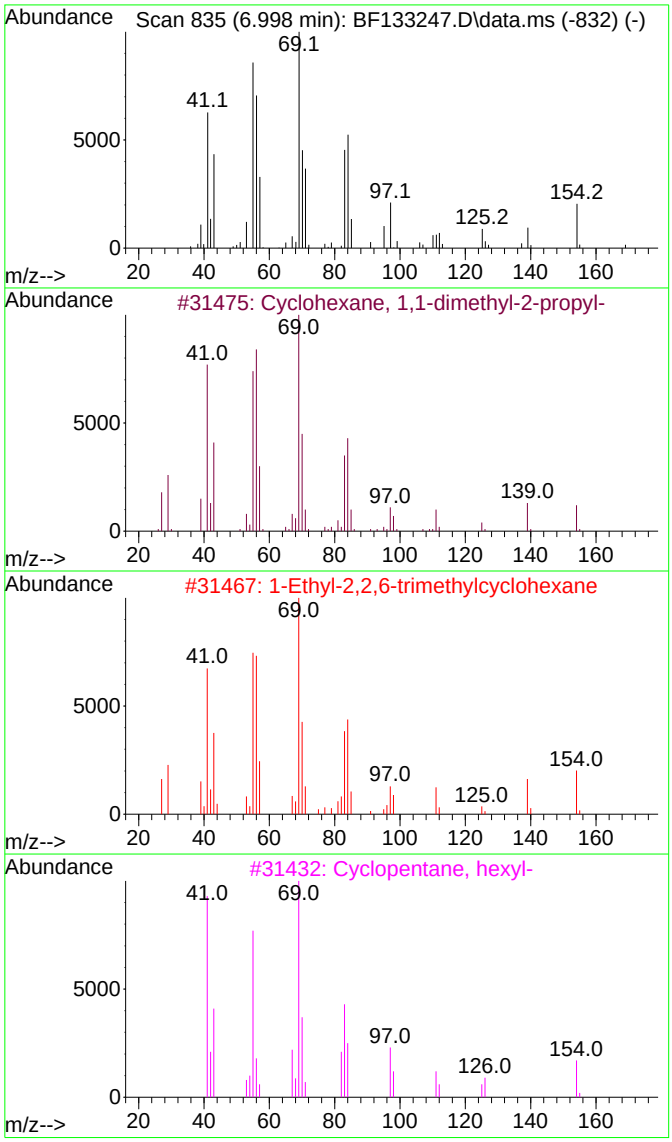
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

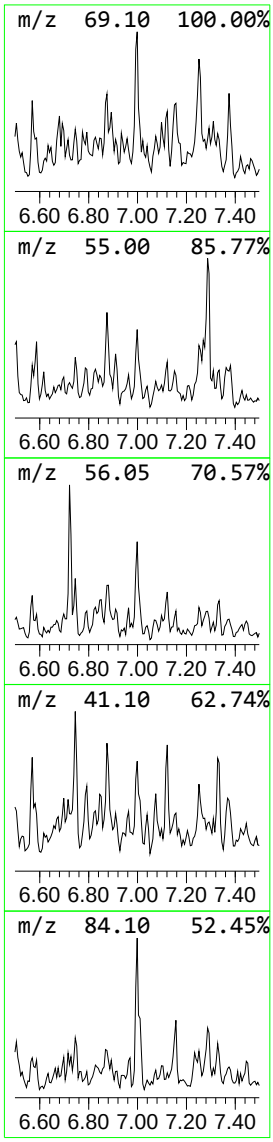
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclohexane, 1,1-dimethyl-2... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.998	2.23 ng	131600	1,4-Dichlorobenzene-d4	6.722

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,1-dimethyl-2-propyl-	154	C11H22	081983-71-3	90
2	1-Ethyl-2,2,6-trimethylcyclohexane	154	C11H22	071186-27-1	90
3	Cyclopentane, hexyl-	154	C11H22	004457-00-5	62
4	1-Heptanol, 4-methyl-	130	C8H18O	000817-91-4	47
5	1-Dodecanol	186	C12H26O	000112-53-8	43





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ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

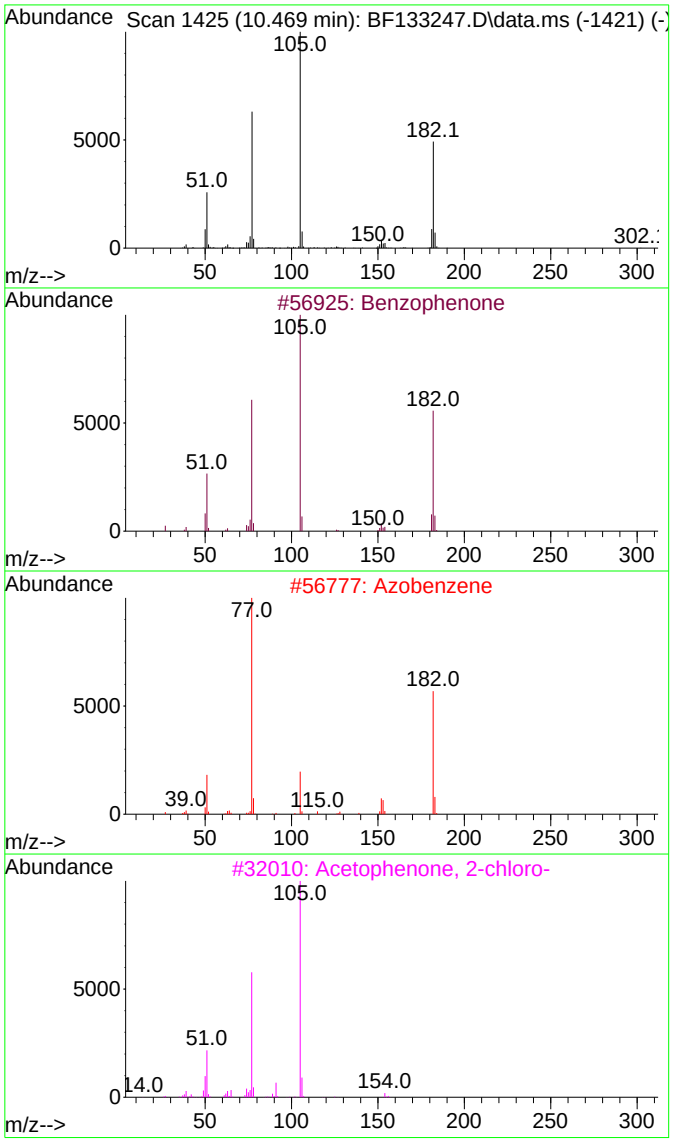
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

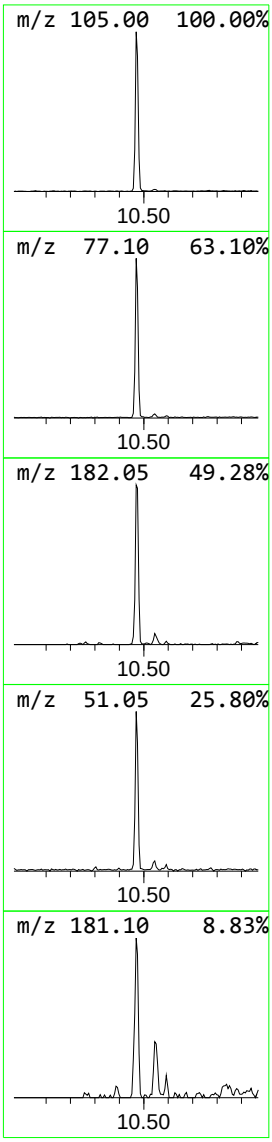
****

Peak Number 4 Benzophenone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.469	3.70 ng	308558	Acenaphthene-d10	9.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Azobenzene	182	C12H10N2	000103-33-3	72
3	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
4	Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	49
5	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050423\
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Misc :
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

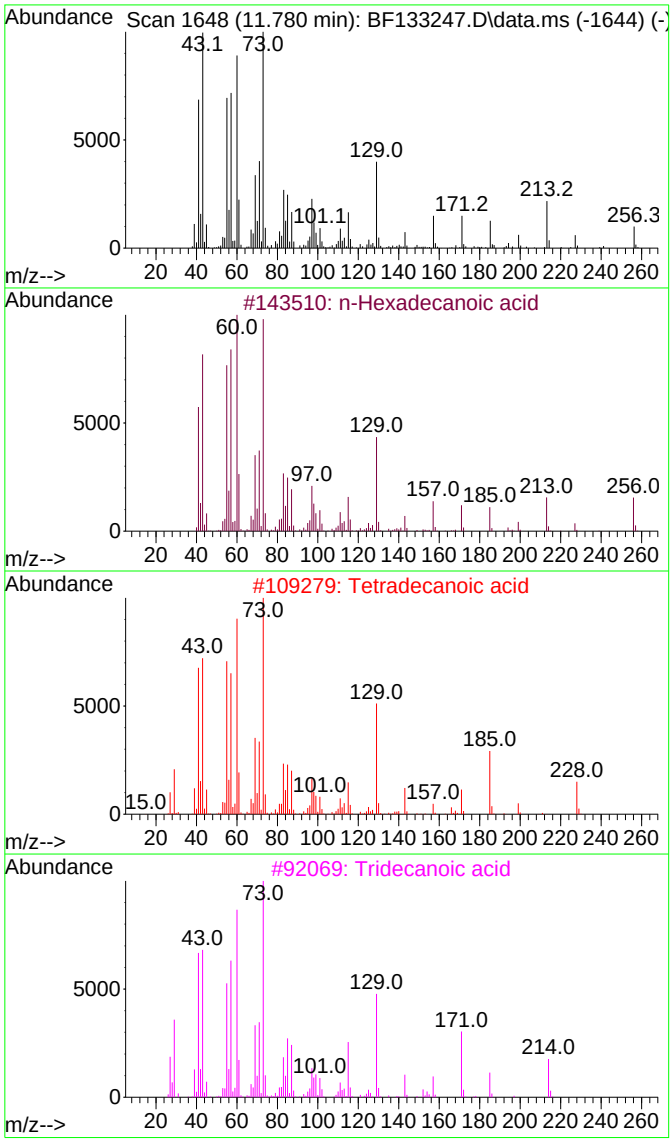
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

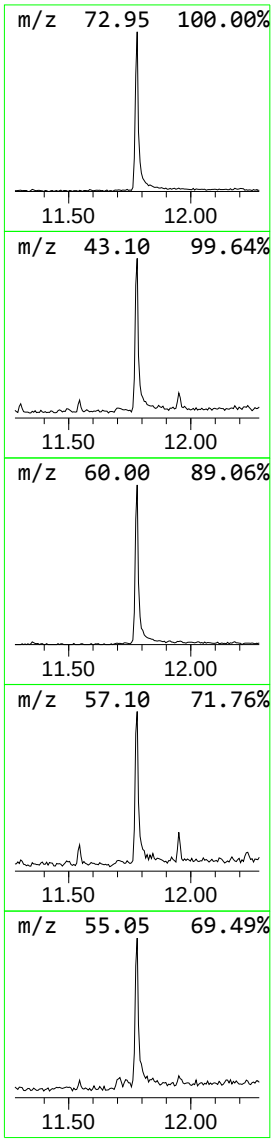
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.780	6.05 ng	478224	Phenanthrene-d10	11.239

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	94
3	Tridecanoic acid	214	C13H26O2	000638-53-9	92
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

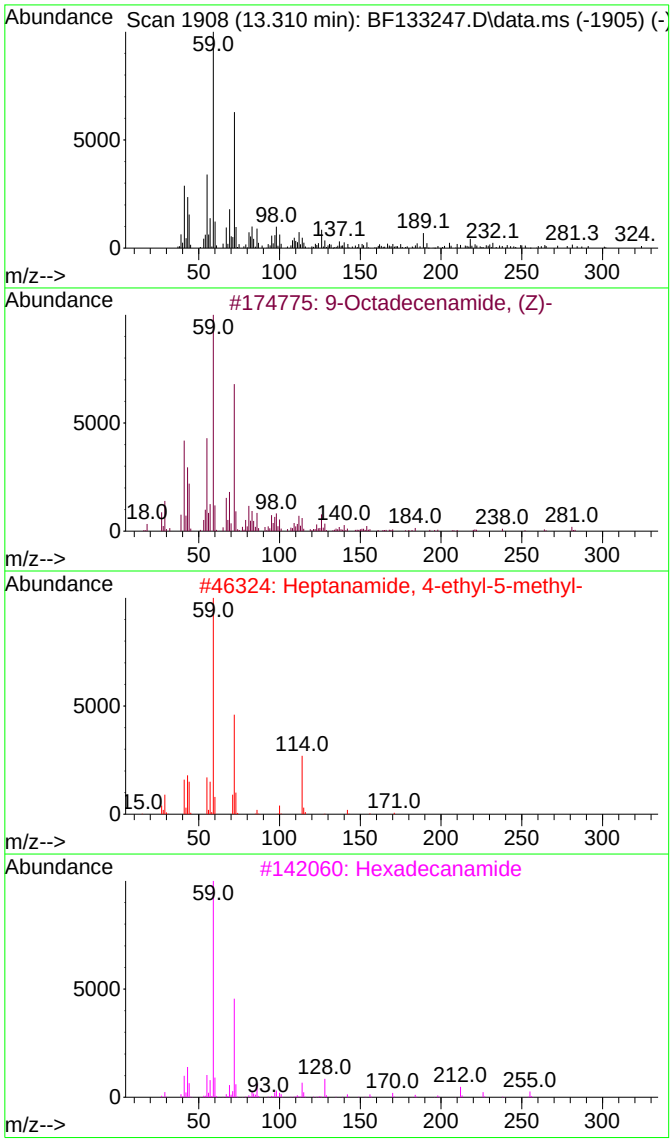
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

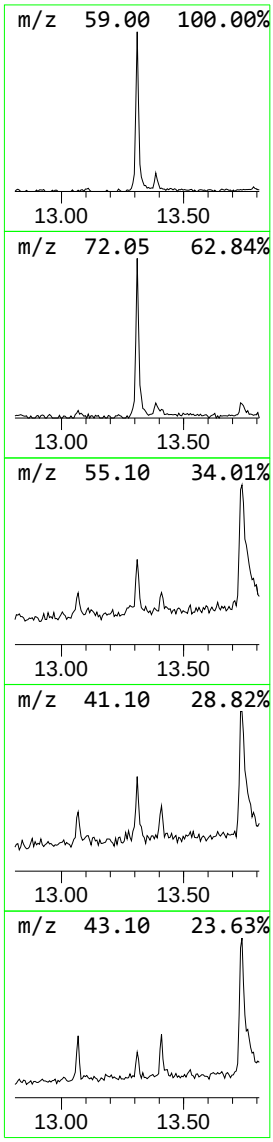
****

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.310	2.18 ng	145148	Chrysene-d12	13.874

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	97
2	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	74
3	Hexadecanamide	255	C16H33NO	000629-54-9	72
4	Octadecanamide	283	C18H37NO	000124-26-5	64
5	Nonanamide	157	C9H19NO	001120-07-6	59





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

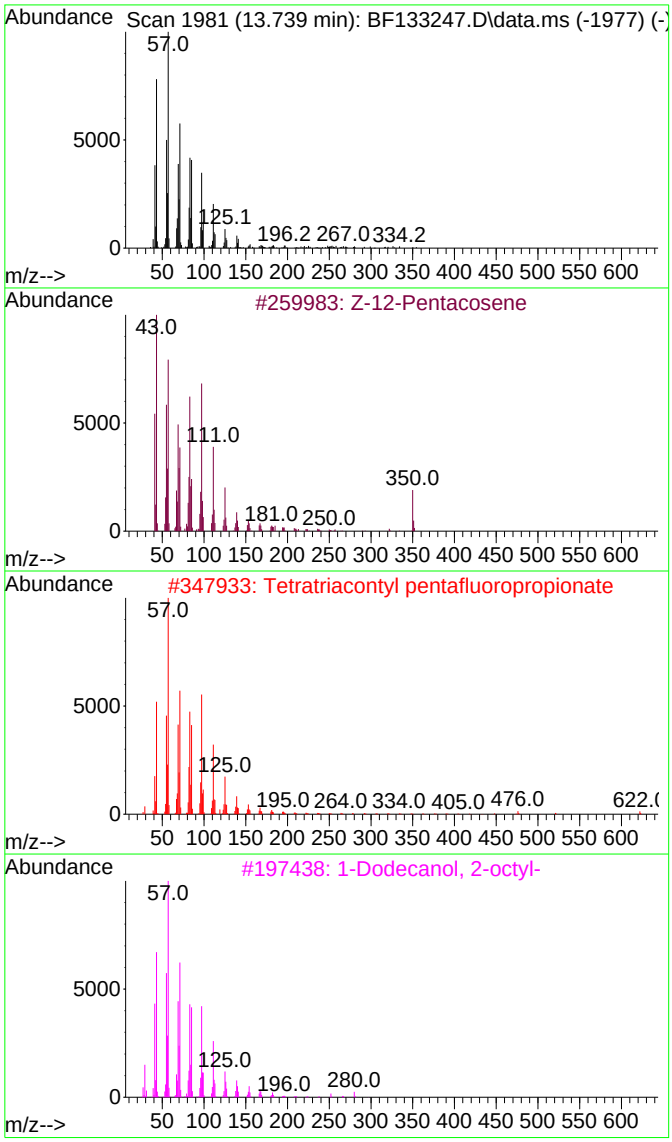
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

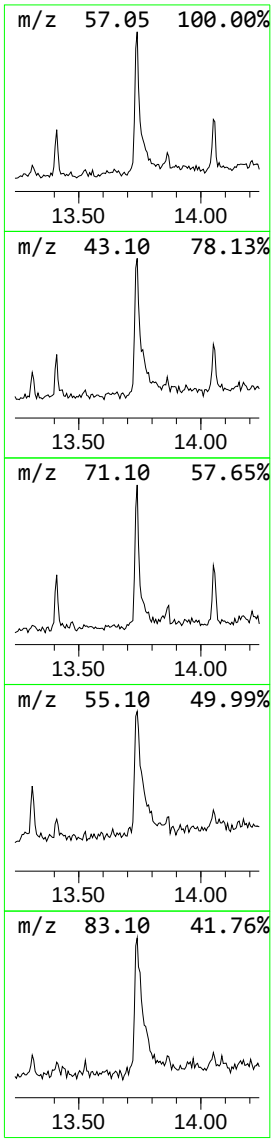
****

Peak Number 7 Z-12-Pentacosene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.739	6.96 ng	462691	Chrysene-d12	13.874

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Z-12-Pentacosene	350	C25H50	1000131-09-4	93
2	Tetratriacontyl pentafluoropropi...	641	C37H69F5O2	1000351-81-5	91
3	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	91
4	Dotriacontyl heptafluorobutyrate	662	C36H65F7O2	1000351-84-2	91
5	Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	91





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Data File : BF133247.D
Acq On : 04 May 2023 23:41
Operator : CG\JU
Sample : 02588-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ZONE-C-0-3-05012023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

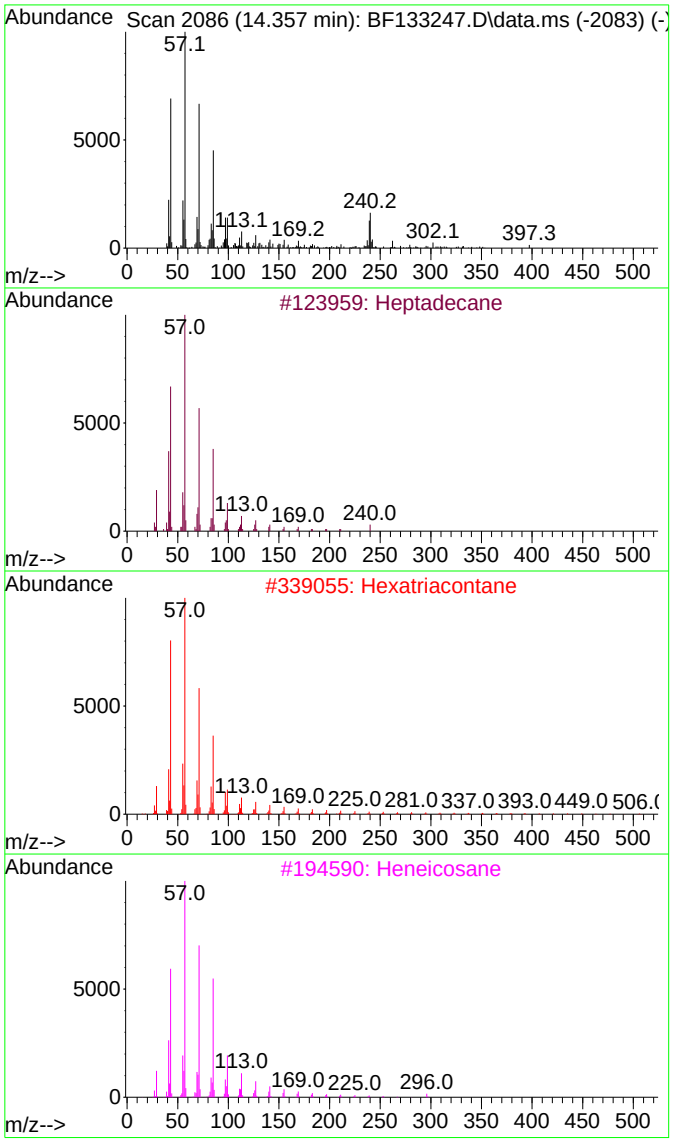
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

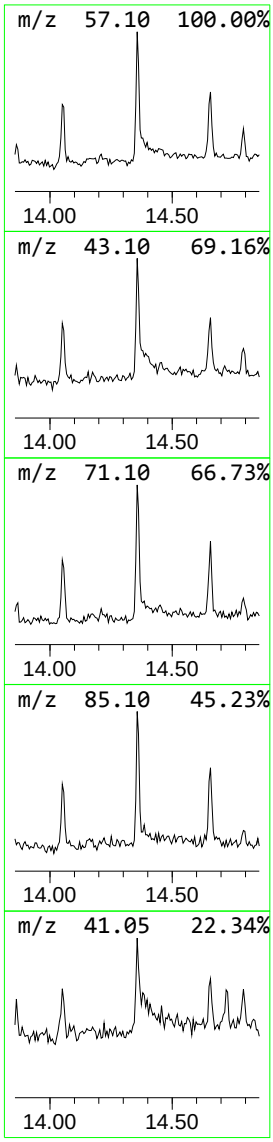
****

Peak Number 8 Heptadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.357	2.17 ng	144548	Chrysene-d12	13.874

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	90
2	Hexatriacontane	507	C36H74	000630-06-8	81
3	Heneicosane	296	C21H44	000629-94-7	76
4	Hexacosane	366	C26H54	000630-01-3	76
5	Octacosane	394	C28H58	000630-02-4	76





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Data File : BF133247.D
Acq On : 04 May 2023 23:41
Operator : CG\JU
Sample : 02588-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ZONE-C-0-3-05012023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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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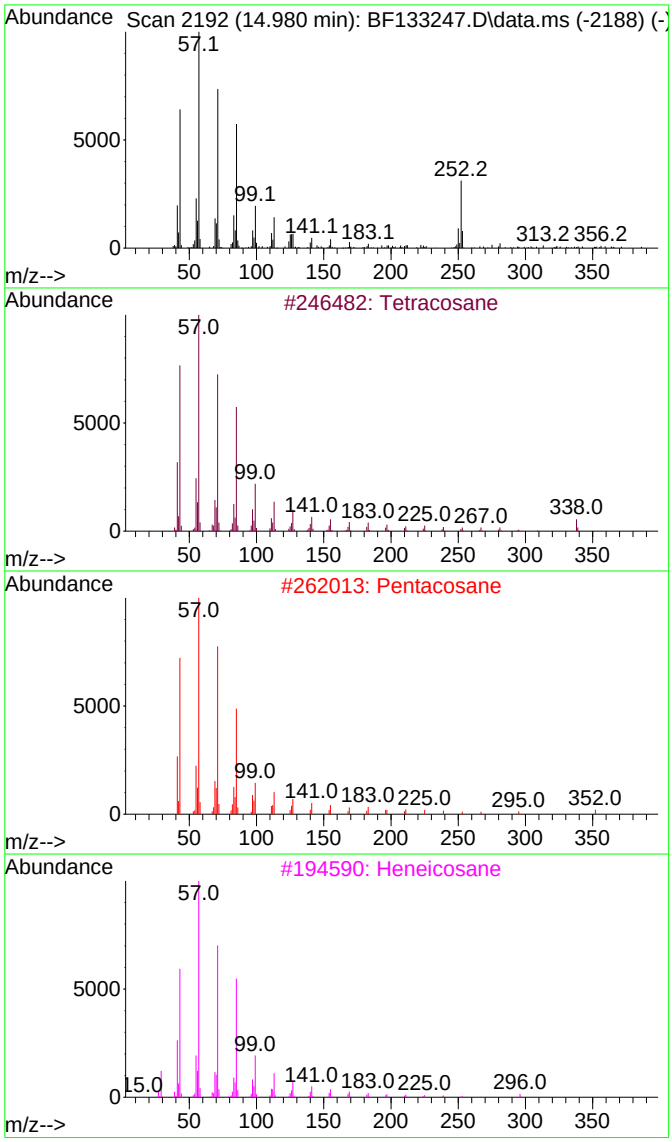
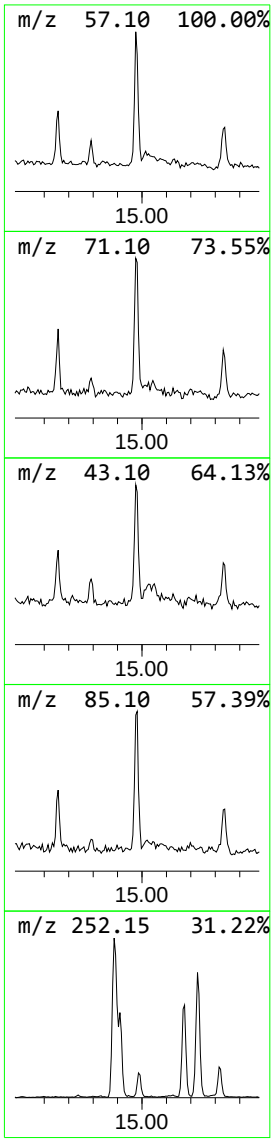
Peak Number 9 Tetracosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.980	3.97 ng	210113	Perylene-d12	15.292

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	90
2	Pentacosane	352	C25H52	000629-99-2	89
3	Heneicosane	296	C21H44	000629-94-7	81
4	Hexacosane, 1-iodo-	492	C26H53I	1000406-32-1	74
5	Octadecane	254	C18H38	000593-45-3	74





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Acq On : 04 May 2023 23:41
Operator : CG\JU
Sample : 02588-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
ZONE-C-0-3-05012023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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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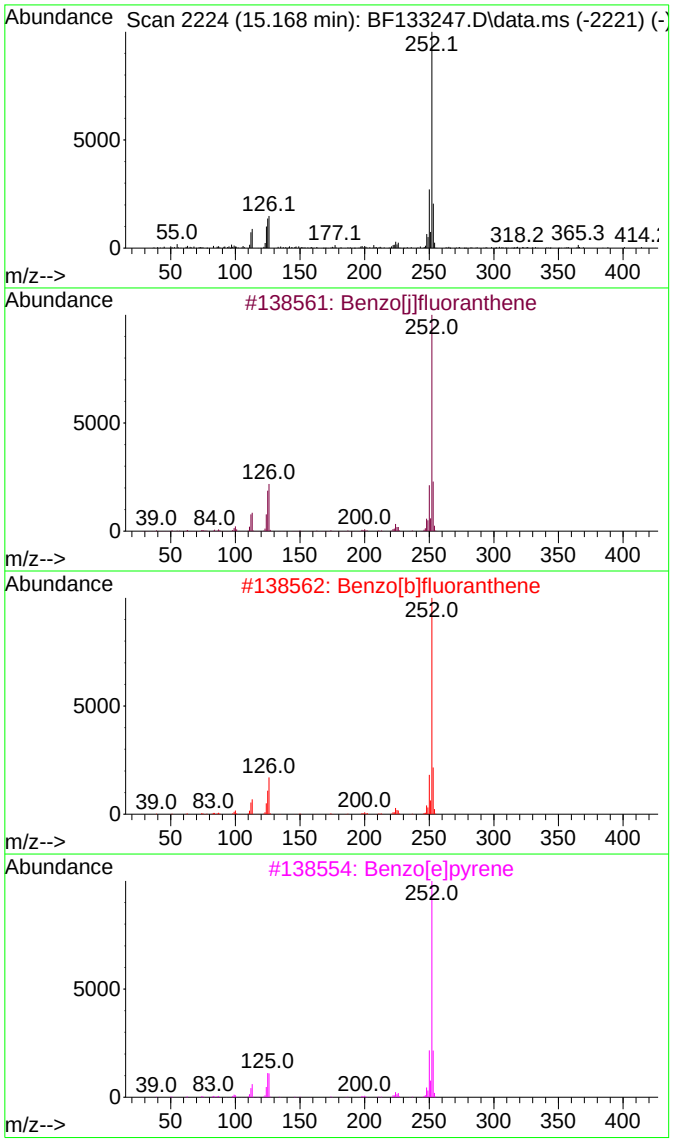
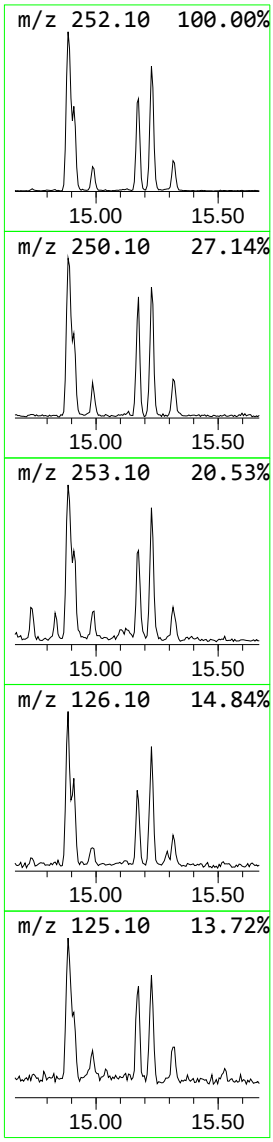
Peak Number 10 Benzo[j]fluoranthene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.168	3.69 ng	195293	Perylene-d12	15.292

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[j]fluoranthene	252	C20H12	000205-82-3	98
2	Benzo[b]fluoranthene	252	C20H12	000205-99-2	98
3	Benzo[e]pyrene	252	C20H12	000192-97-2	98
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	94
5	Perylene	252	C20H12	000198-55-0	93





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Acq On : 04 May 2023 23:41
Operator : CG\JU
Sample : 02588-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
ZONE-C-0-3-05012023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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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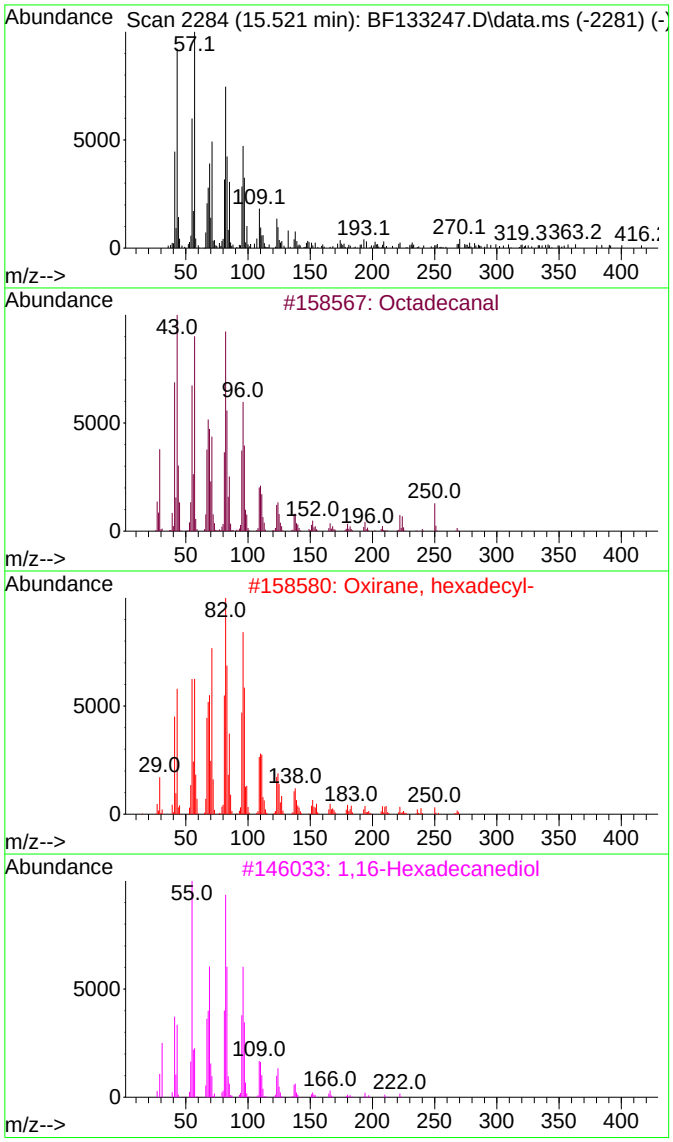
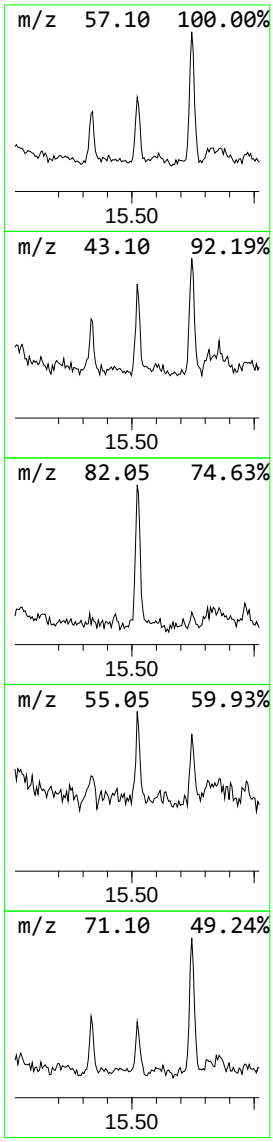
Peak Number 11 Octadecanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.521	3.83 ng	202417	Perylene-d12	15.292

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	91
2	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
3	1,16-Hexadecanediol	258	C16H34O2	007735-42-4	68
4	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	68
5	(Z)-14-Tricosenyl formate	366	C24H46O2	077899-10-6	64





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Data File : BF133247.D
Acq On : 04 May 2023 23:41
Operator : CG\JU
Sample : 02588-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ZONE-C-0-3-05012023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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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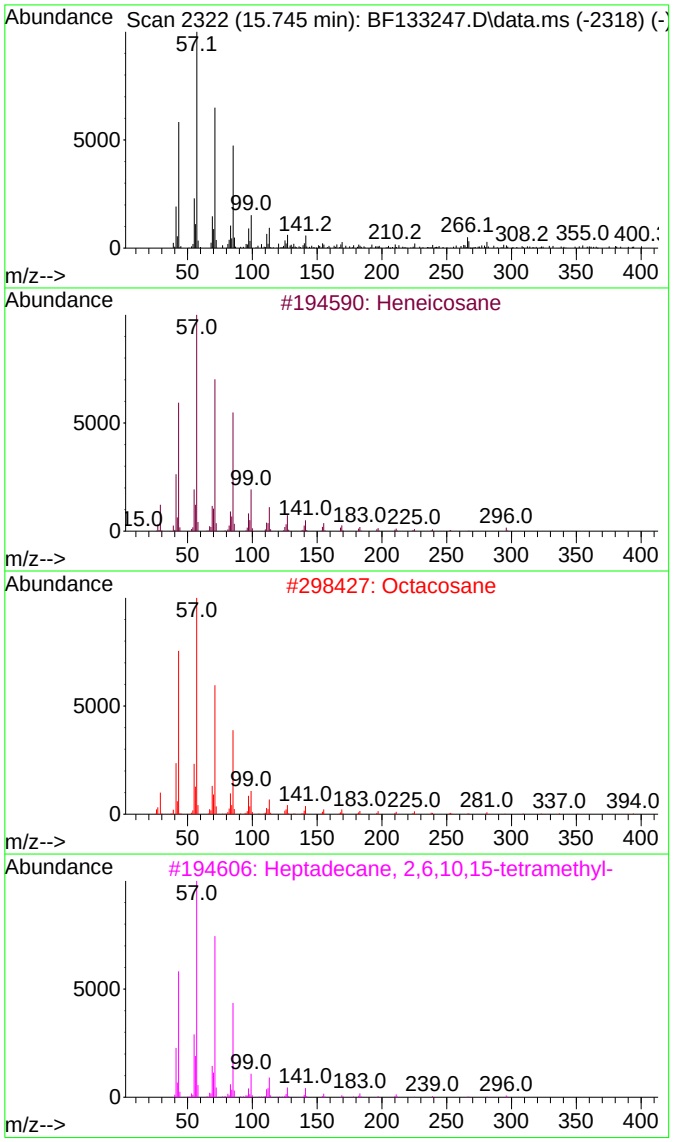
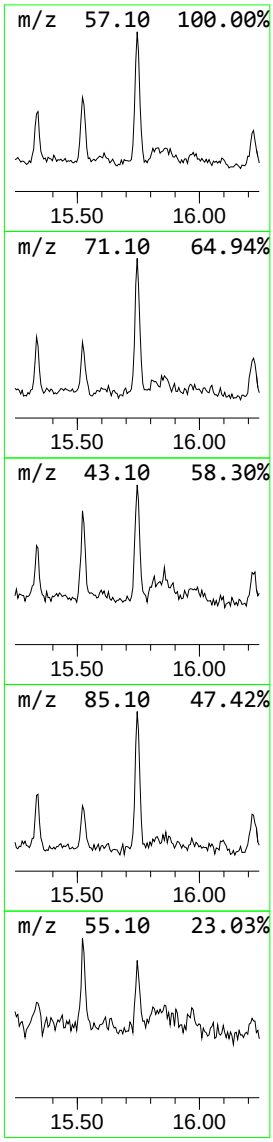
Peak Number 12 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.745	4.00 ng	211571	Perylene-d12	15.292

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	93
2	Octacosane	394	C28H58	000630-02-4	93
3	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	91
4	Hentriacontane	437	C31H64	000630-04-6	90
5	Heptacosane	380	C27H56	000593-49-7	89





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Data File : BF133247.D
Acq On : 04 May 2023 23:41
Operator : CG\JU
Sample : 02588-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ZONE-C-0-3-05012023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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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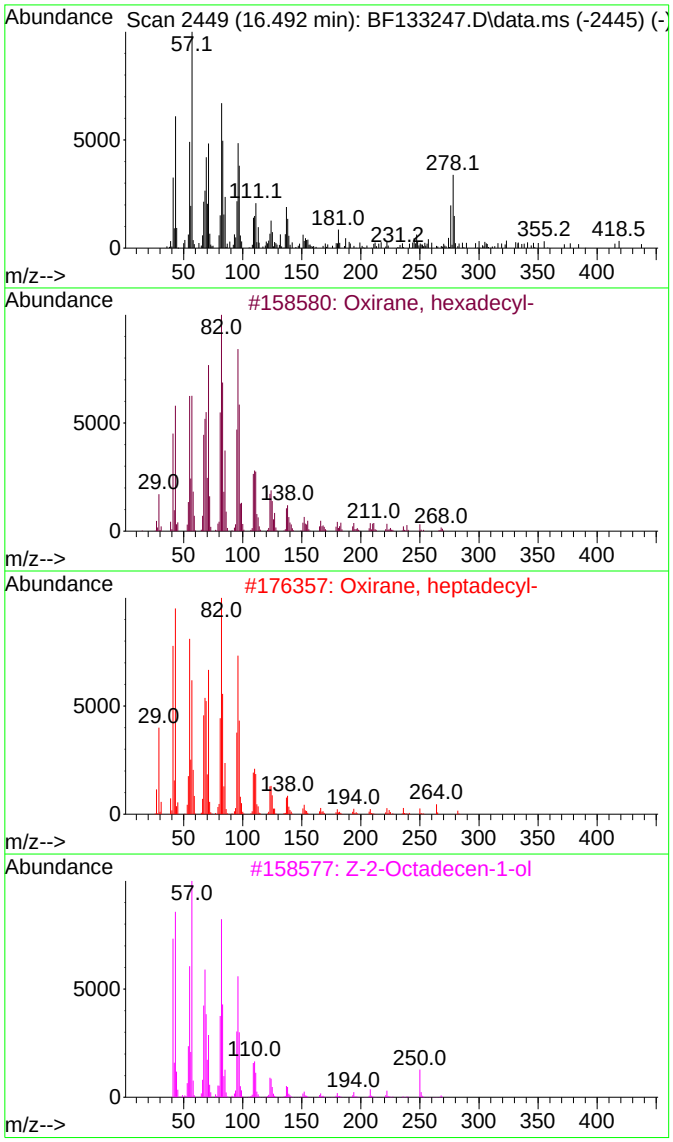
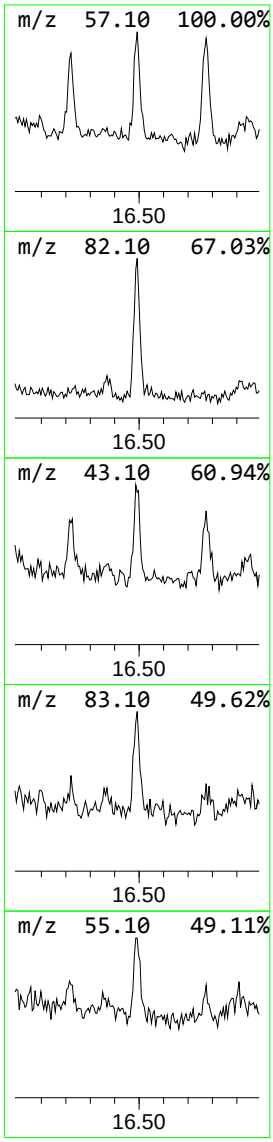
Peak Number 13 Oxirane, hexadecyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.492	3.95 ng	208698	Perylene-d12	15.292

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	93
2	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	55
3	Z-2-Octadecen-1-ol	268	C18H36O	1000131-11-0	49
4	Hexacosanal	380	C26H52O	026627-85-0	38
5	Cyclopentane, (4-octyldodecyl)-	350	C25H50	005638-09-5	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050423\
Data File : BF133247.D
Acq On : 04 May 2023 23:41
Operator : CG\JU
Sample : 02588-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ZONE-C-0-3-05012023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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
Cyclohexane, 1,...	6.257	4.0	ng	236837	1	6.722	1182880	20.0
Cyclohexane, 1,...	6.998	2.2	ng	131600	1	6.722	1182880	20.0
Benzophenone	10.469	3.7	ng	308558	3	9.757	1667700	20.0
n-Hexadecanoic ...	11.780	6.0	ng	478224	4	11.239	1580000	20.0
9-Octadecenamid...	13.310	2.2	ng	145148	5	13.874	1330200	20.0
Z-12-Pentacosene	13.739	7.0	ng	462691	5	13.874	1330200	20.0
Heptadecane	14.357	2.2	ng	144548	5	13.874	1330200	20.0
Tetracosane	14.980	4.0	ng	210113	6	15.292	1057500	20.0
Benzo[j]fluoran...	15.168	3.7	ng	195293	6	15.292	1057500	20.0
Octadecanal	15.521	3.8	ng	202417	6	15.292	1057500	20.0
Heneicosane	15.745	4.0	ng	211571	6	15.292	1057500	20.0
Oxirane, hexade...	16.492	4.0	ng	208698	6	15.292	1057500	20.0