LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092424\
Data File : BF139525.D
Acq On : 24 Sep 2024 17:35
Operator : RC/JU
Sample : P4149-14
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-7

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-BF091324.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139525.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.069	497	506	515	rVB	47957	69878	5.74%	0.619%
2	5.487	567	577	587	rBV	768441	1017712	83.61%	9.019%
3	6.498	744	749	768	rVB	812505	1060144	87.10%	9.395%
4	6.875	808	813	818	rVB	261193	310111	25.48%	2.748%
5	7.433	899	908	913	rBV	545111	675092	55.46%	5.983%
6	7.692	946	952	959	rVB3	7504	12648	1.04%	0.112%
7	8.157	1026	1031	1038	rBV	331404	410287	33.71%	3.636%
8	9.227	1208	1213	1224	rBV	936238	1186515	97.48%	10.515%
9	9.910	1324	1329	1333	rBV	381062	459549	37.76%	4.072%
10	10.621	1443	1450	1458	rBV	77688	96792	7.95%	0.858%
11	10.698	1458	1463	1473	rBV	523880	665656	54.69%	5.899%
12	10.933	1494	1503	1507	rBV	11507	14820	1.22%	0.131%
13	11.398	1577	1582	1590	rBV2	408205	668136	54.89%	5.921%
14	11.468	1590	1594	1598	rVB	22285	28200	2.32%	0.250%
15	11.627	1618	1621	1628	rVB	10837	14846	1.22%	0.132%
16	11.898	1662	1667	1668	rBV	19192	22439	1.84%	0.199%
17	11.921	1668	1671	1677	rVB2	38673	56939	4.68%	0.505%
18	12.010	1682	1686	1695	rVB2	45978	82249	6.76%	0.729%
19	12.186	1709	1716	1719	rBV2	14390	25595	2.10%	0.227%
20	12.216	1719	1721	1726	rVB2	11635	13652	1.12%	0.121%
21	12.445	1757	1760	1763	rBV	10695	13353	1.10%	0.118%
22	12.521	1768	1773	1780	rVB4	32739	58591	4.81%	0.519%
23	12.610	1783	1788	1792	rVB	179941	225647	18.54%	2.000%
24	12.657	1792	1796	1800	rBV5	11009	16639	1.37%	0.147%
25	12.704	1800	1804	1807	rBV2	42419	56020	4.60%	0.496%
26	12.739	1807	1810	1816	rVB3	19066	28770	2.36%	0.255%
27	12.839	1816	1827	1832	rBV	158337	262321	21.55%	2.325%
28	12.980	1844	1851	1858	rVB	943703	1217162	100.00%	10.786%
29	13.068	1859	1866	1870	rBV5	18782	45296	3.72%	0.401%
30	13.163	1875	1882	1886	rVV2	54257	75196	6.18%	0.666%
31	13.198	1886	1888	1892	rVV2	19442	24093	1.98%	0.214%
32	13.268	1896	1900	1903	rVV2	18112	25306	2.08%	0.224%
33	13.298	1903	1905	1908	rVV2	15964	16422	1.35%	0.146%
34	13.351	1911	1914	1918	rBV2	43076	54469	4.48%	0.483%
35	13.392	1918	1921	1926	rVV3	19580	29072	2.39%	0.258%
36	13.457	1926	1932	1941	rVV	310015	443714	36.45%	3.932%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092424\
Data File : BF139525.D
Acq On : 24 Sep 2024 17:35
Operator : RC/JU
Sample : P4149-14
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-7

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-BF091324.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.562	1945	1950	1958	rVB4	26826	58277	4.79%	0.516%
38	13.668	1964	1968	1973	rVB	35710	45673	3.75%	0.405%
39	13.780	1983	1987	1990	rBV2	22442	33122	2.72%	0.294%
40	13.880	2001	2004	2010	rVB	25985	40293	3.31%	0.357%
41	14.033	2023	2030	2042	rVB2	361848	662737	54.45%	5.873%
42	14.192	2054	2057	2061	rBV3	9331	13073	1.07%	0.116%
43	14.421	2092	2096	2099	rBV	15434	20322	1.67%	0.180%
44	14.498	2106	2109	2114	rBV5	14705	20481	1.68%	0.182%
45	14.545	2115	2117	2124	rVB6	8773	14498	1.19%	0.128%
46	14.662	2134	2137	2141	rVB4	14226	18402	1.51%	0.163%
47	14.886	2171	2175	2179	rBV2	24427	38633	3.17%	0.342%
48	15.074	2202	2207	2216	rBV	91849	211082	17.34%	1.871%
49	15.180	2223	2225	2230	rVB	11784	14585	1.20%	0.129%
50	15.380	2254	2259	2265	rVB	46065	71516	5.88%	0.634%
51	15.439	2265	2269	2275	rVV	55877	86423	7.10%	0.766%
52	15.504	2275	2280	2293	rVB	202001	358688	29.47%	3.179%
53	16.974	2524	2530	2540	rVB2	22219	48938	4.02%	0.434%
54	17.421	2600	2606	2617	rVB2	18389	44174	3.63%	0.391%

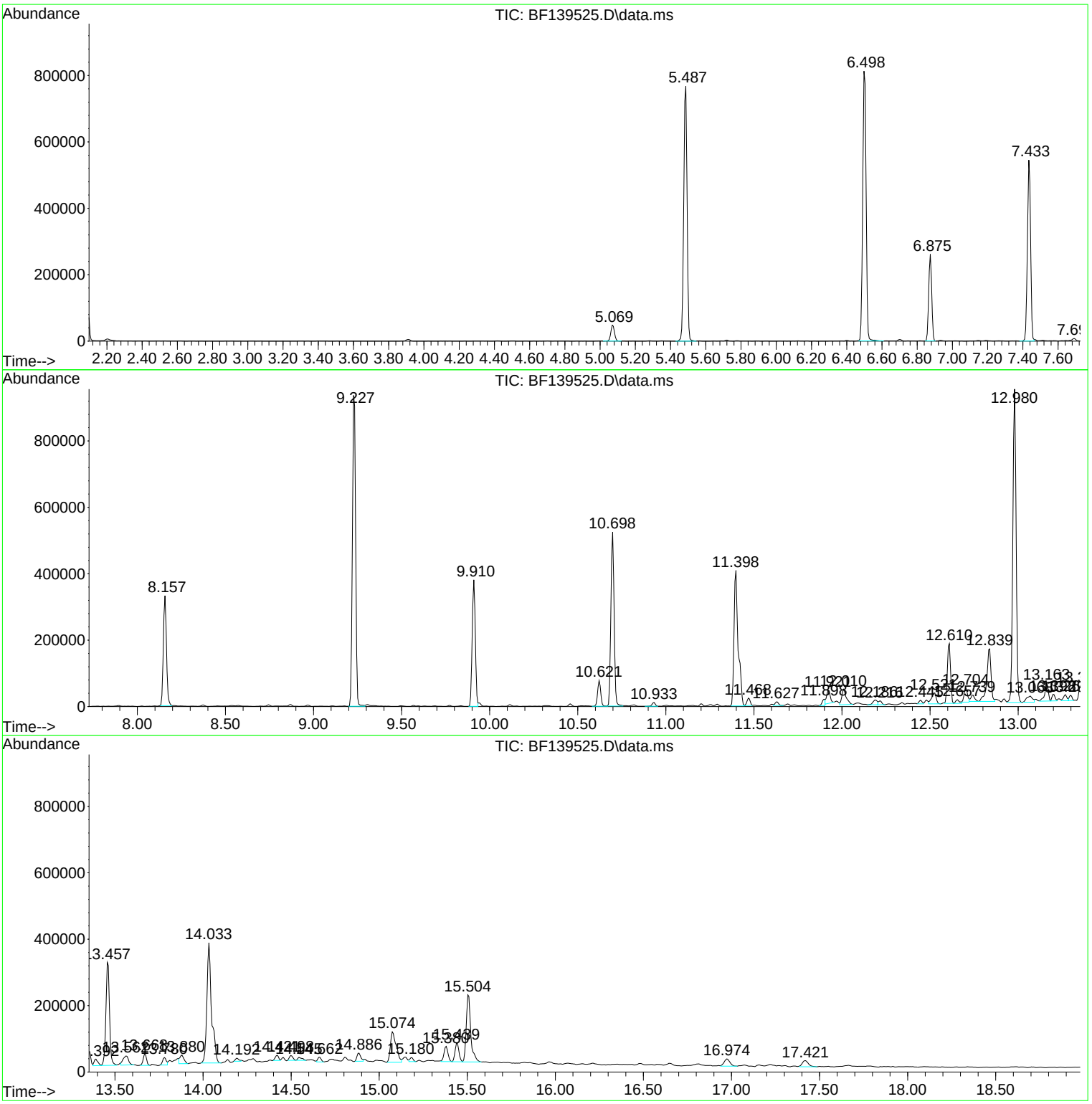
Sum of corrected areas: 11284248

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092424\
Data File : BF139525.D
Acq On : 24 Sep 2024 17:35
Operator : RC/JU
Sample : P4149-14
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092424\
Data File : BF139525.D
Acq On : 24 Sep 2024 17:35
Operator : RC/JU
Sample : P4149-14
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.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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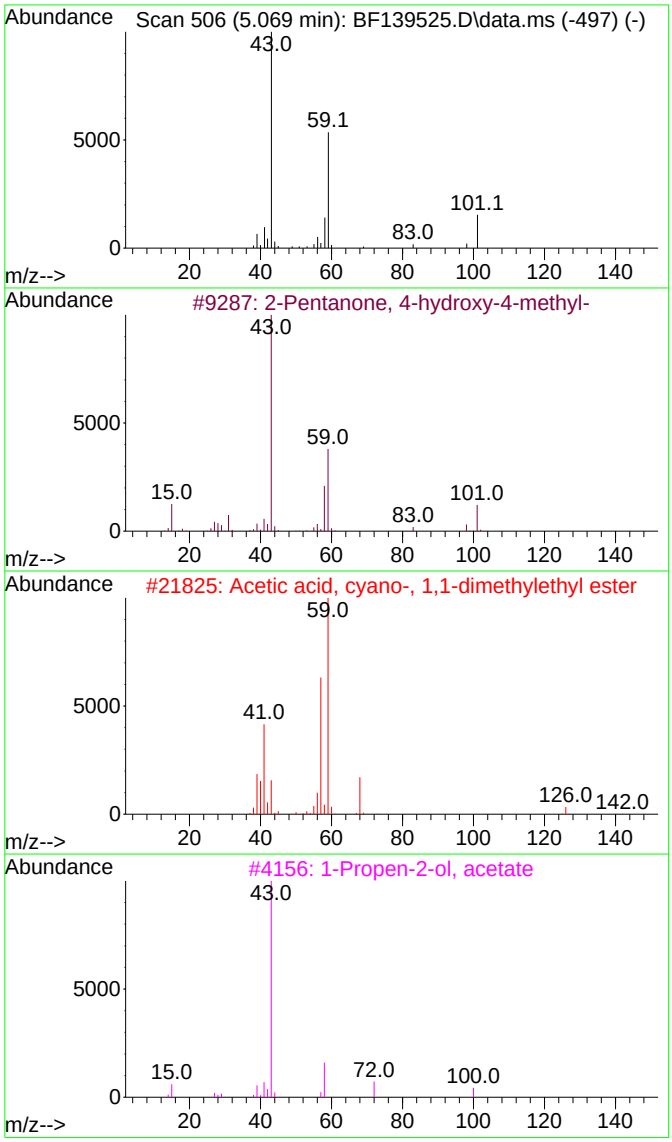
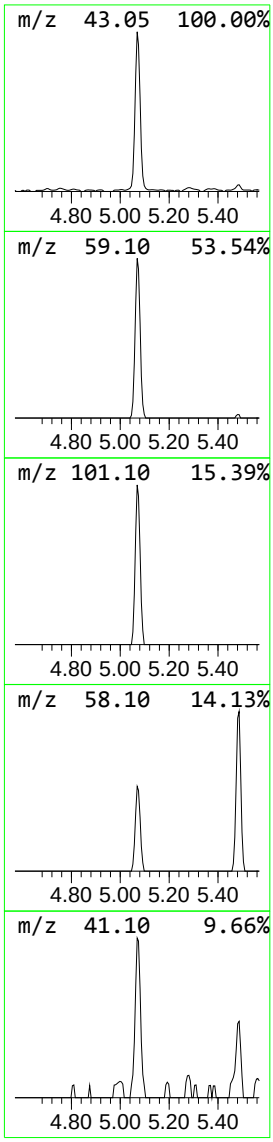
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.069	4.51 ng	69878	1,4-Dichlorobenzene-d4	6.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Diacetamide	101	C4H7NO2	000625-77-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092424\
Data File : BF139525.D
Acq On : 24 Sep 2024 17:35
Operator : RC/JU
Sample : P4149-14
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.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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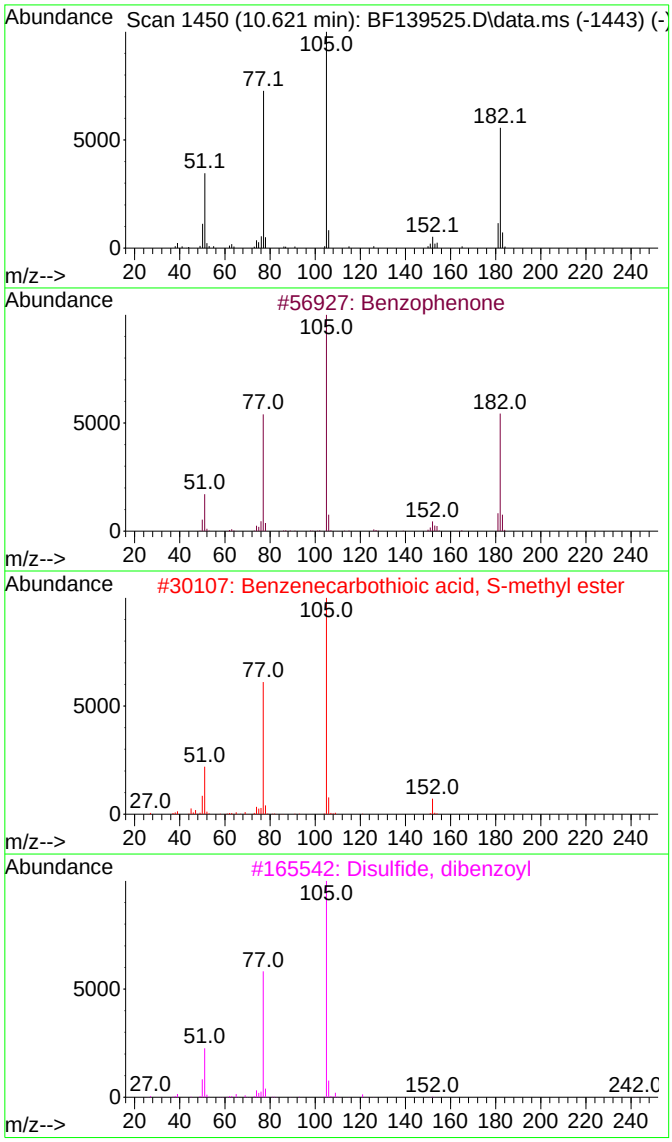
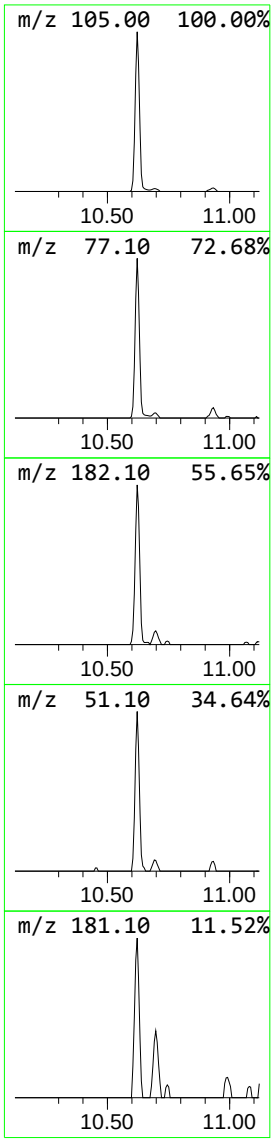
Peak Number 2 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.621	4.21 ng	96792	Acenaphthene-d10	9.910

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	64
3	Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	47
4	1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47
5	N-cyanobenzamide	146	C8H6N2O	015150-25-1	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092424\
Data File : BF139525.D
Acq On : 24 Sep 2024 17:35
Operator : RC/JU
Sample : P4149-14
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.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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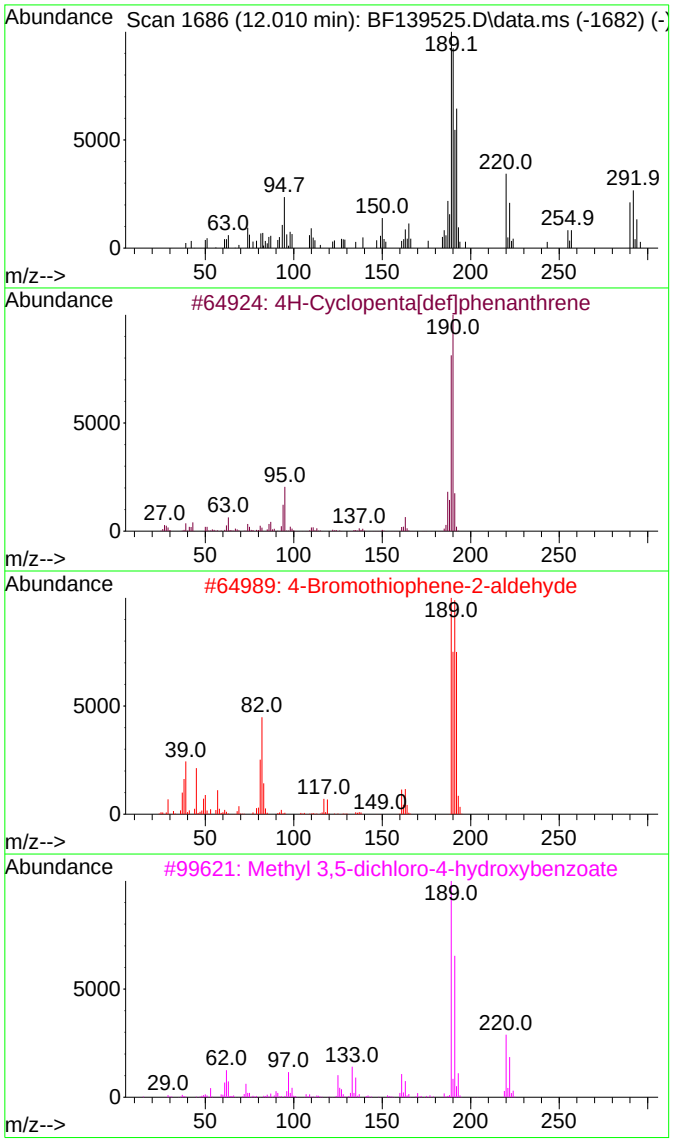
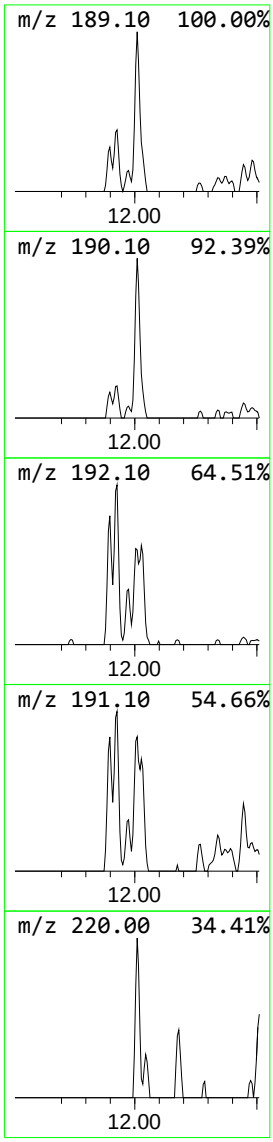
Peak Number 3 unknown12.010 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.010	2.46 ng	82249	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	45
2	4-Bromothiophene-2-aldehyde	190	C5H3BrOS	018791-75-8	43
3	Methyl 3,5-dichloro-4-hydroxyben...	220	C8H6Cl2O3	003337-59-5	43
4	1-(4-Fluorophenyl)-4,5-dimethyli...	190	C11H11FN2	1000443-18-7	43
5	2,4-Dichloro-3-fluorobenzonitrile	189	C7H2Cl2FN	161612-68-6	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092424\
Data File : BF139525.D
Acq On : 24 Sep 2024 17:35
Operator : RC/JU
Sample : P4149-14
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.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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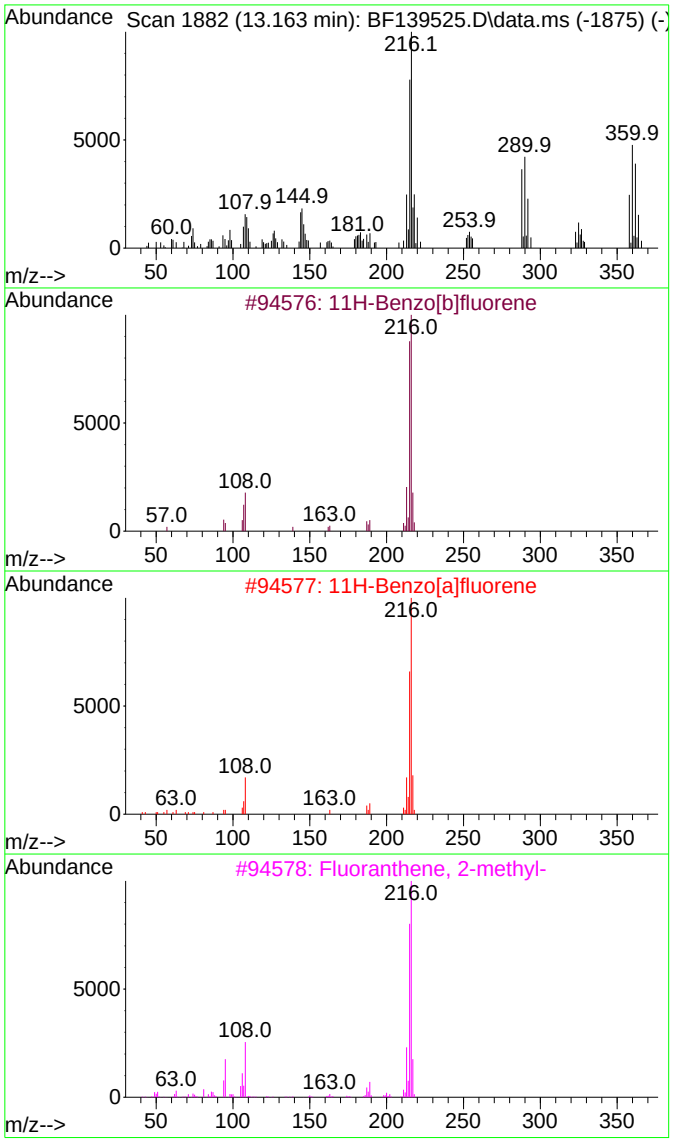
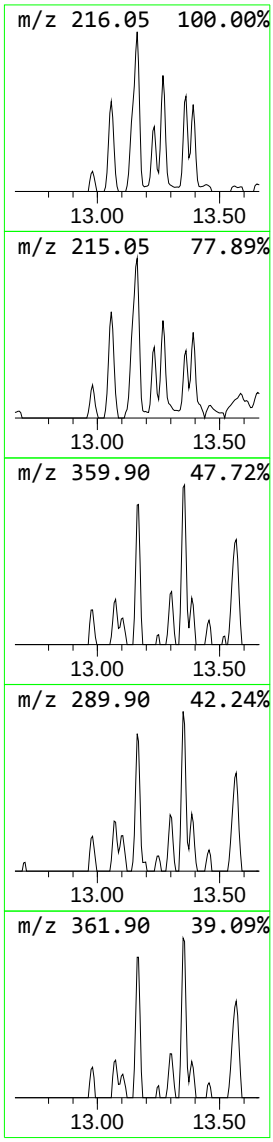
Peak Number 4 11H-Benzo[b]fluorene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.163	2.27 ng	75196	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	89
2	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	83
3	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	46
4	Pyrene, 1-methyl-	216	C17H12	002381-21-7	46
5	1-Pyrenebutanoic acid	288	C20H16O2	003443-45-6	18





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Data File : BF139525.D
Acq On : 24 Sep 2024 17:35
Operator : RC/JU
Sample : P4149-14
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.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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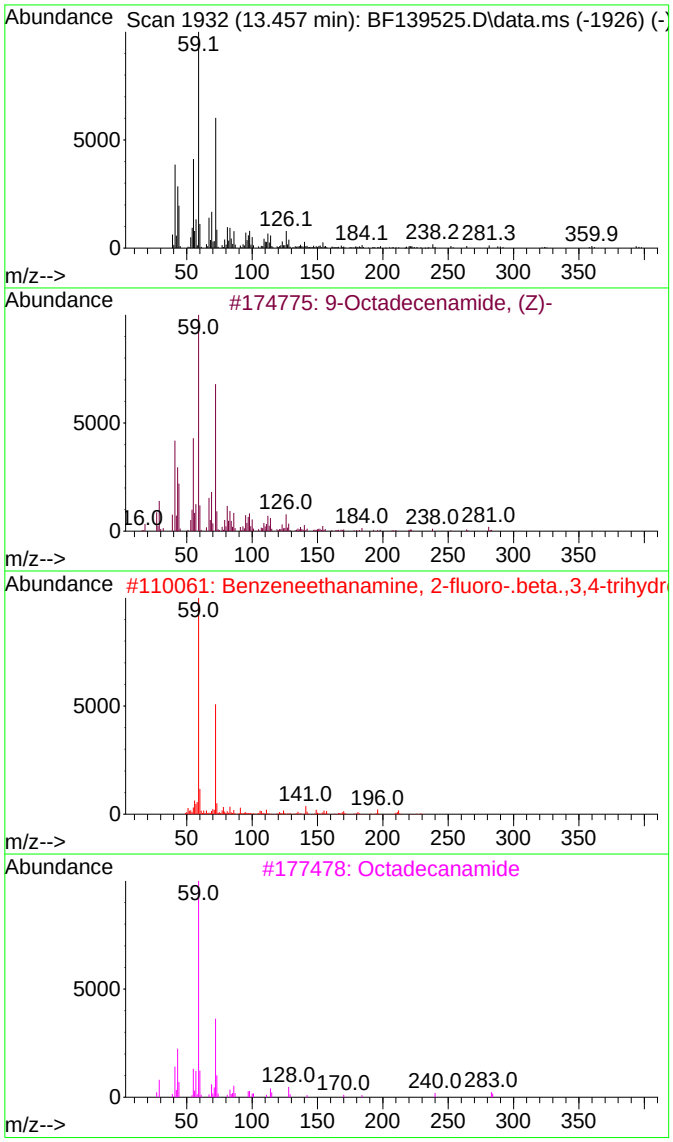
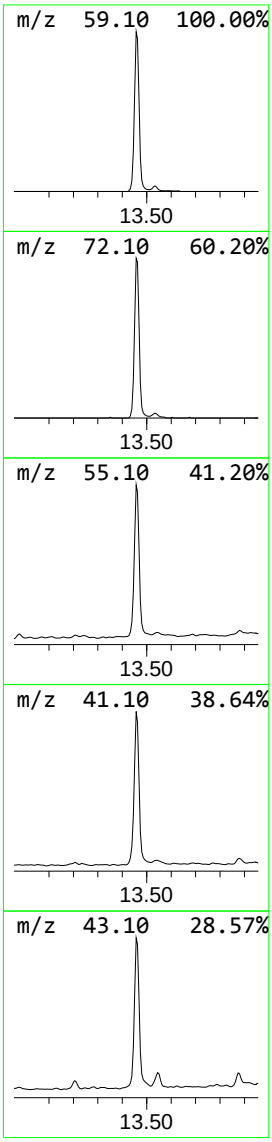
Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.457	13.39 ng	443714	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	98
2	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	53
3	Octadecanamide	283	C18H37NO	000124-26-5	53
4	Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	53
5	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092424\
Data File : BF139525.D
Acq On : 24 Sep 2024 17:35
Operator : RC/JU
Sample : P4149-14
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.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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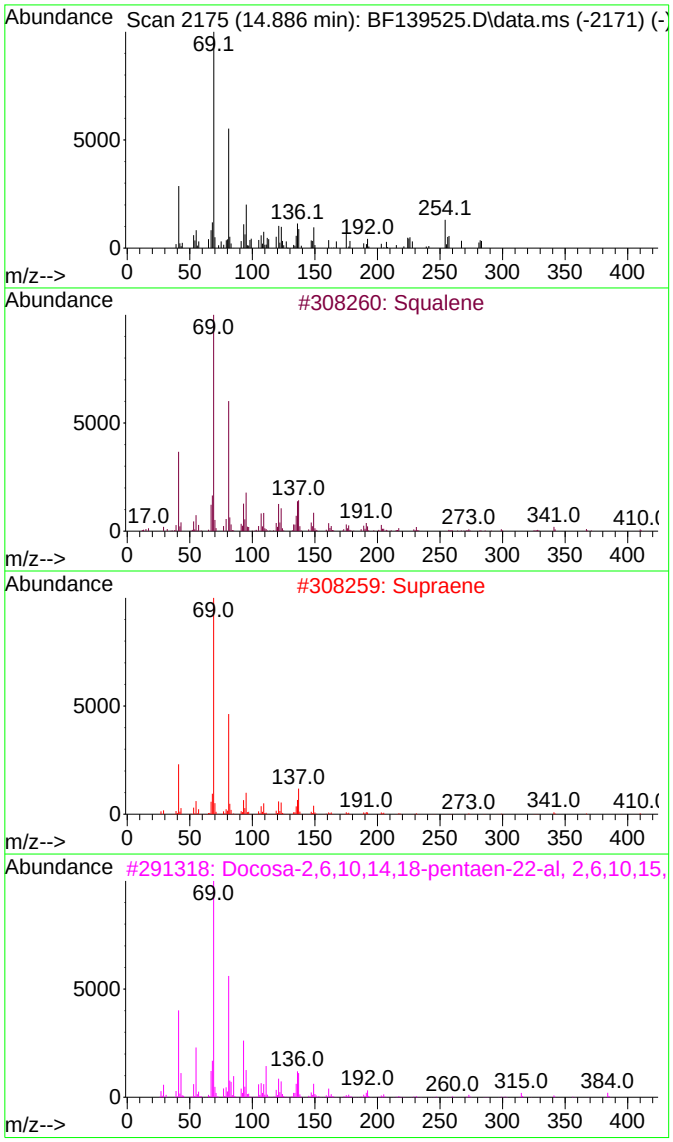
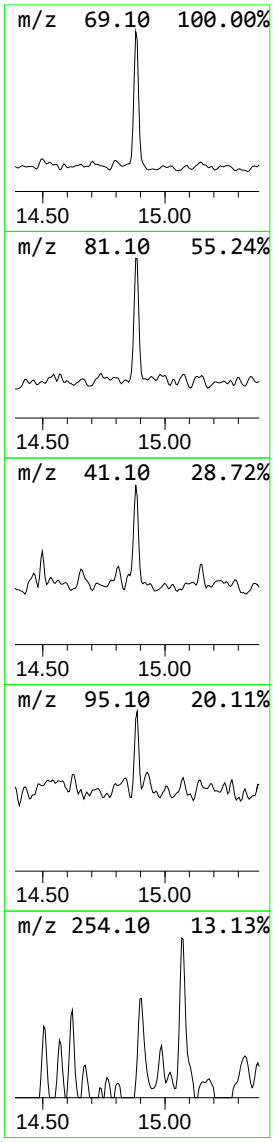
Peak Number 6 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.886	2.15 ng	38633	Perylene-d12	15.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	74
2	Supraene	410	C30H50	007683-64-9	64
3	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	64
4	5,9,13-Pentadecatrien-2-one, 6,1...	262	C18H30O	000762-29-8	59
5	2,6,10,14-Hexadecatetraen-1-ol, ...	332	C22H36O2	061691-98-3	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092424\
Data File : BF139525.D
Acq On : 24 Sep 2024 17:35
Operator : RC/JU
Sample : P4149-14
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.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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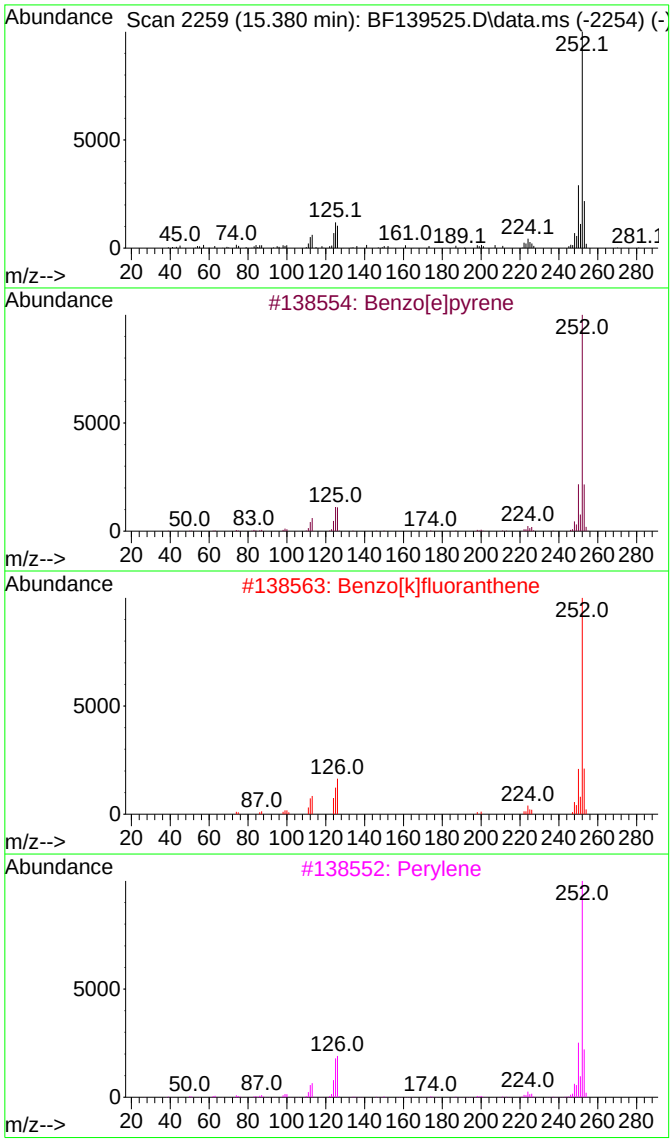
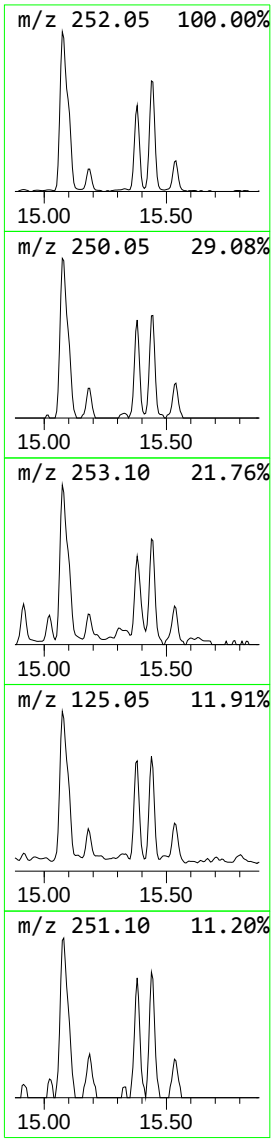
Peak Number 7 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.380	3.99 ng	71516	Perylene-d12	15.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	97
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
3	Perylene	252	C20H12	000198-55-0	95
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	95
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092424\
Data File : BF139525.D
Acq On : 24 Sep 2024 17:35
Operator : RC/JU
Sample : P4149-14
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.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
2-Pentanone, 4-...	5.069	4.5	ng	69878	1	6.875	310111	20.0
Benzophenone	10.621	4.2	ng	96792	3	9.910	459549	20.0
unknown12.010	12.010	2.5	ng	82249	4	11.398	668136	20.0
11H-Benzo[b]flu...	13.163	2.3	ng	75196	5	14.033	662737	20.0
9-Octadecenamid...	13.457	13.4	ng	443714	5	14.033	662737	20.0
Squalene	14.886	2.1	ng	38633	6	15.504	358688	20.0
Benzo[e]pyrene	15.380	4.0	ng	71516	6	15.504	358688	20.0