

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022125\
 Data File : BF141727.D
 Acq On : 21 Feb 2025 18:44
 Operator : RC/JU
 Sample : Q1397-01
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 STOCK-PILE

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-BF020625.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF141727.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.352	379	384	391	rBV	24469	41989	2.10%	0.221%
2	4.987	487	492	508	rVB	41227	71933	3.59%	0.379%
3	5.399	557	562	591	rBV	1165447	1689726	84.41%	8.897%
4	6.416	730	735	764	rBV	1180616	1763399	88.09%	9.285%
5	6.775	791	796	805	rBV	420998	551316	27.54%	2.903%
6	7.340	887	892	904	rBV	795461	1124932	56.19%	5.923%
7	7.610	933	938	958	rVB2	16651	44706	2.23%	0.235%
8	8.063	1009	1015	1032	rBV	497184	736346	36.78%	3.877%
9	9.134	1192	1197	1207	rBV	1573415	2001893	100.00%	10.541%
10	9.210	1207	1210	1222	rVB3	11037	22780	1.14%	0.120%
11	9.675	1284	1289	1294	rBV	16078	21395	1.07%	0.113%
12	9.810	1307	1312	1327	rBV	565539	750558	37.49%	3.952%
13	10.522	1428	1433	1441	rBV	151768	202340	10.11%	1.065%
14	10.598	1441	1446	1462	rVV	696226	985272	49.22%	5.188%
15	10.722	1462	1467	1474	rVB4	12361	27772	1.39%	0.146%
16	11.192	1544	1547	1554	rVB	17526	24728	1.24%	0.130%
17	11.298	1560	1565	1567	rBV	442956	639169	31.93%	3.365%
18	11.375	1574	1578	1582	rVB	31042	39583	1.98%	0.208%
19	11.533	1601	1605	1611	rBV2	27519	49073	2.45%	0.258%
20	11.798	1646	1650	1651	rBV	39294	43782	2.19%	0.231%
21	11.828	1651	1655	1665	rVV2	342352	567850	28.37%	2.990%
22	11.910	1665	1669	1678	rVB2	85319	169283	8.46%	0.891%
23	12.092	1697	1700	1703	rBV	23459	30954	1.55%	0.163%
24	12.122	1703	1705	1710	rVB	36209	45557	2.28%	0.240%
25	12.345	1739	1743	1746	rBV	34048	47687	2.38%	0.251%
26	12.380	1746	1749	1755	rVB3	26530	43293	2.16%	0.228%
27	12.433	1755	1758	1765	rVB	39211	60602	3.03%	0.319%
28	12.510	1765	1771	1776	rBV	588340	766883	38.31%	4.038%
29	12.610	1784	1788	1793	rBV2	99950	162675	8.13%	0.857%
30	12.739	1803	1810	1815	rBV	514650	766064	38.27%	4.034%
31	12.786	1815	1818	1823	rVB2	28974	44172	2.21%	0.233%
32	12.880	1827	1834	1842	rBV	1149058	1533537	76.60%	8.075%
33	12.957	1842	1847	1851	rBV3	44839	78464	3.92%	0.413%
34	13.063	1858	1865	1869	rVB	75222	150948	7.54%	0.795%
35	13.133	1873	1877	1879	rVV	40412	53826	2.69%	0.283%
36	13.169	1879	1883	1890	rVB2	61682	100257	5.01%	0.528%

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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-BF020625.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.263	1895	1899	1901	rVV	31515	36785	1.84%	0.194%
38	13.292	1901	1904	1912	rVB2	33140	51053	2.55%	0.269%
39	13.574	1949	1952	1958	rVB	51726	71810	3.59%	0.378%
40	13.686	1966	1971	1973	rBV	61802	93355	4.66%	0.492%
41	13.786	1984	1988	1991	rBV	36935	46187	2.31%	0.243%
42	13.933	2006	2013	2016	rBV2	575844	1065757	53.24%	5.612%
43	14.086	2036	2039	2043	rBV4	23244	39463	1.97%	0.208%
44	14.133	2043	2047	2051	rVV2	64732	87607	4.38%	0.461%
45	14.286	2069	2073	2076	rBV2	51760	82180	4.11%	0.433%
46	14.404	2090	2093	2097	rVB3	26033	39705	1.98%	0.209%
47	14.445	2098	2100	2102	rBV	20671	25051	1.25%	0.132%
48	14.963	2182	2188	2196	rBV	275674	620226	30.98%	3.266%
49	15.068	2202	2206	2210	rBV	31713	40916	2.04%	0.215%
50	15.251	2233	2237	2243	rVB	120297	188865	9.43%	0.994%
51	15.316	2243	2248	2253	rVV	185363	272304	13.60%	1.434%
52	15.374	2253	2258	2273	rVB2	255128	490574	24.51%	2.583%
53	16.804	2495	2501	2509	rVB2	78203	164908	8.24%	0.868%
54	17.233	2568	2574	2583	rBV	54933	120613	6.02%	0.635%

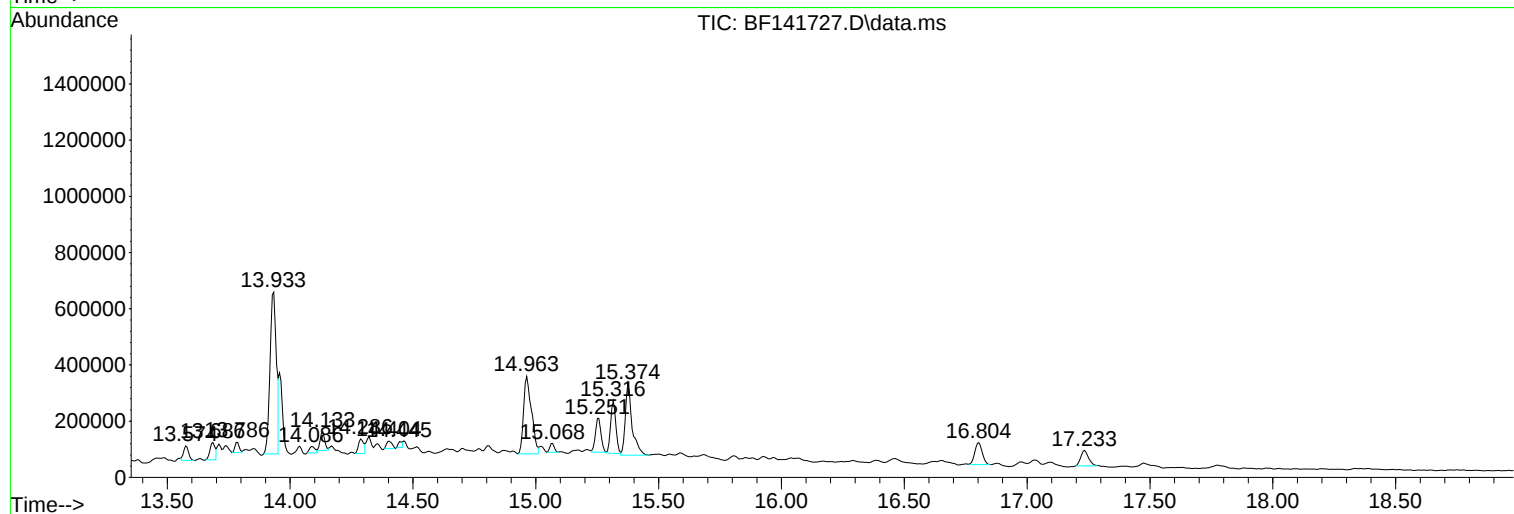
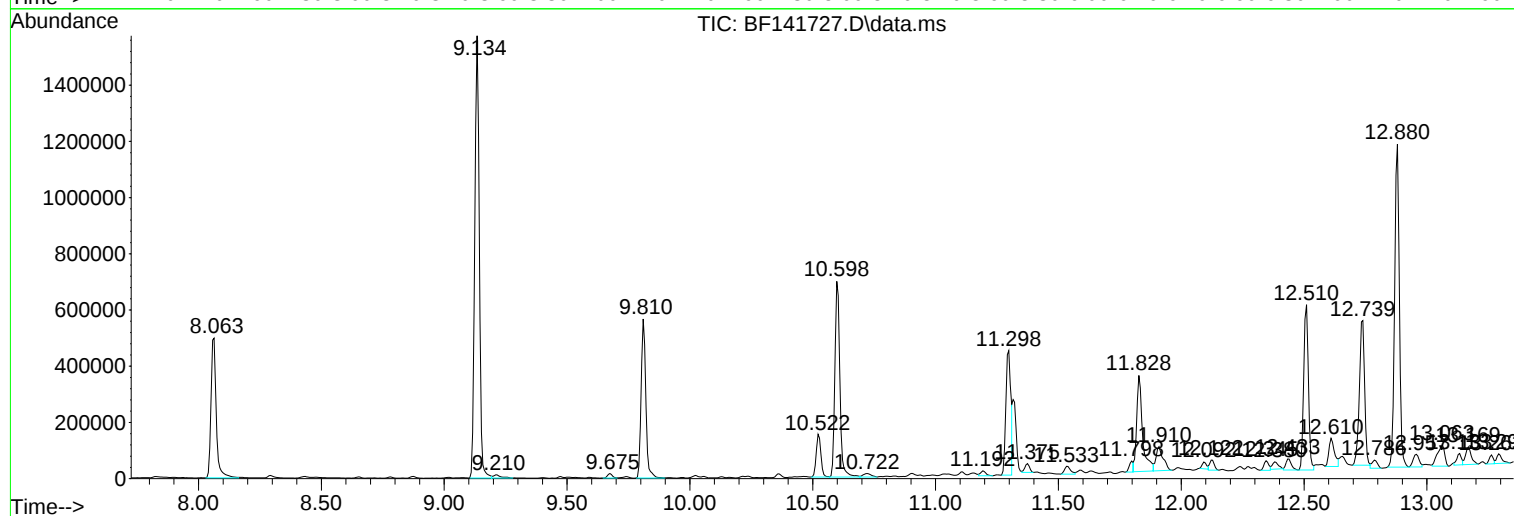
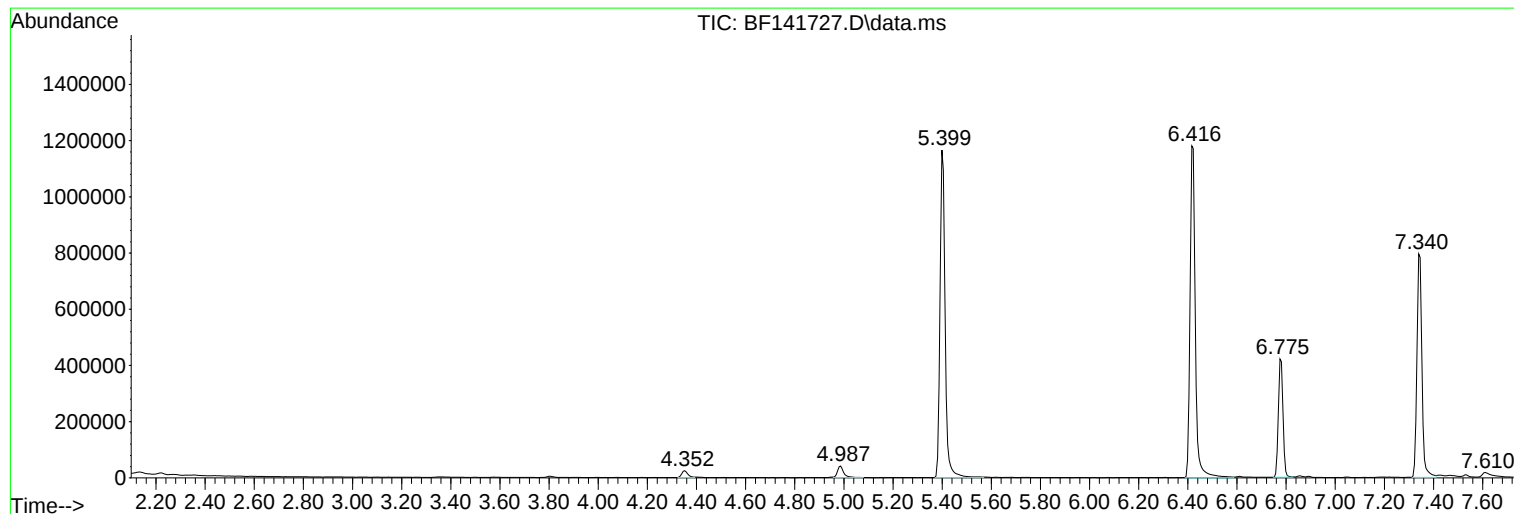
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020625.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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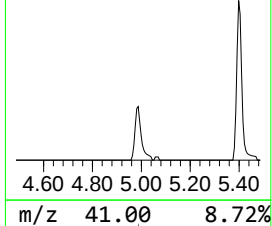
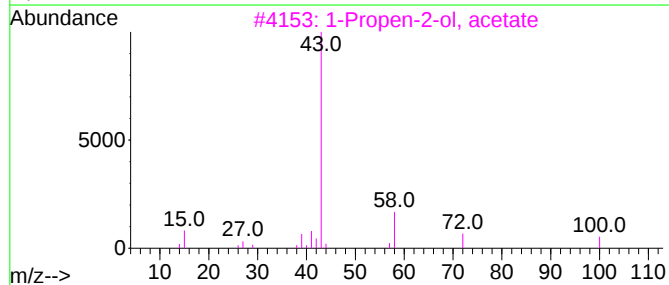
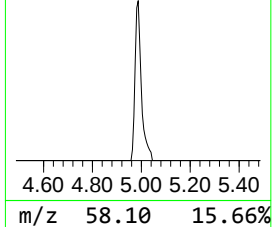
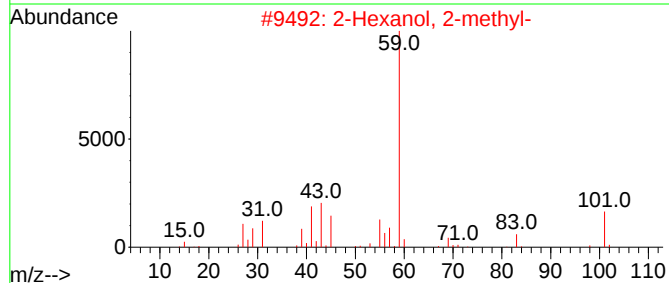
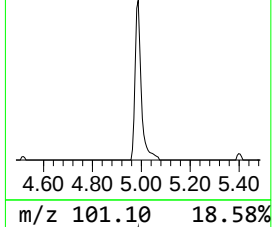
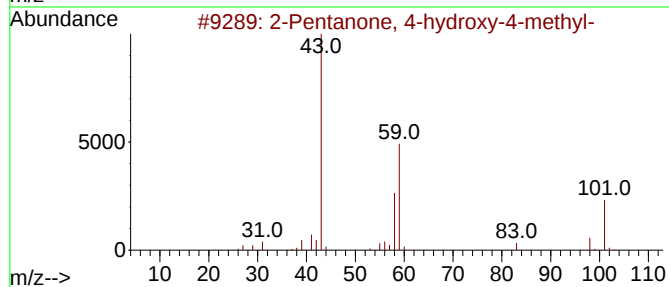
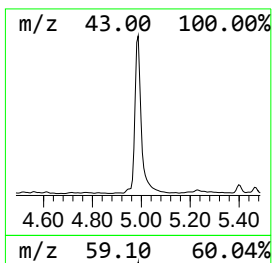
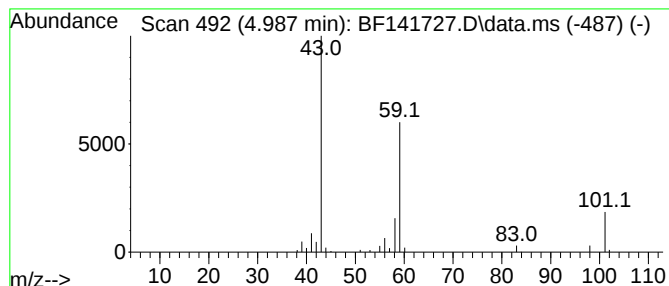
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.987	2.61 ng	71933	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		



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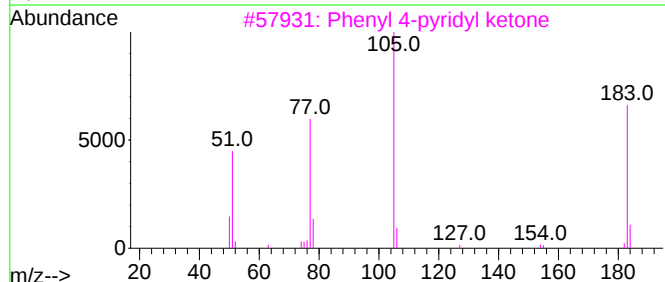
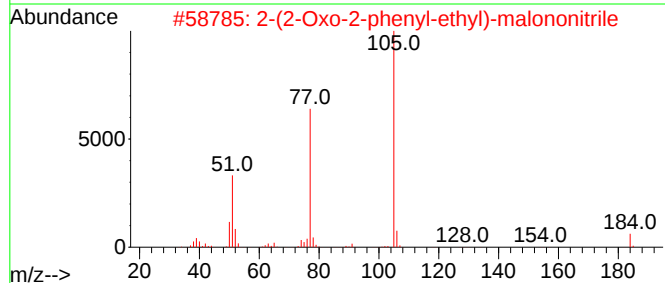
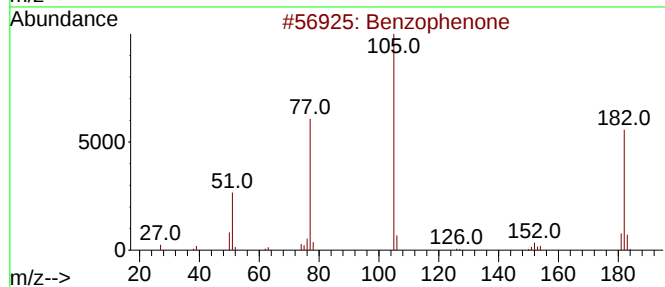
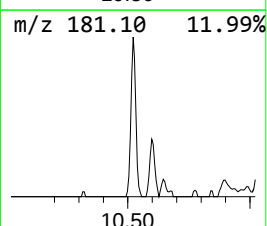
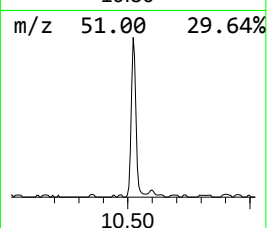
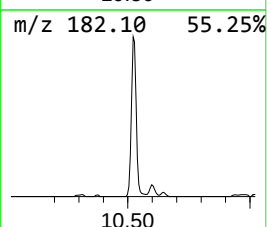
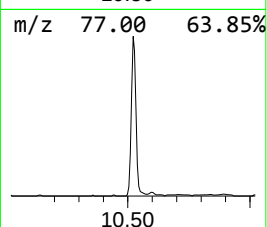
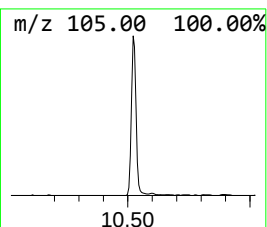
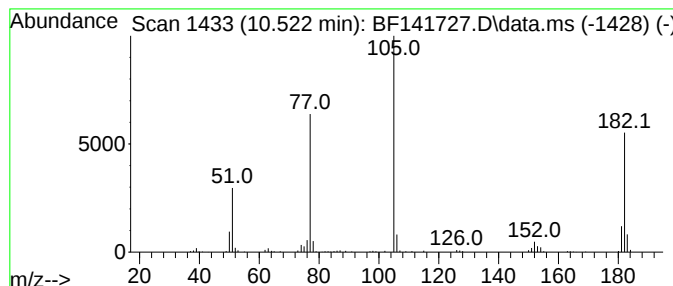
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.522	5.39 ng	202340	Acenaphthene-d10	9.810

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	53
3			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	49
4			acetic acid, 2-bromo-, 2-oxo-2-p...	256	C10H9BrO3	1000401-50-0	47
5			Pentafluoroethyl phenyl ketone	224	C9H5F5O	000394-52-5	47



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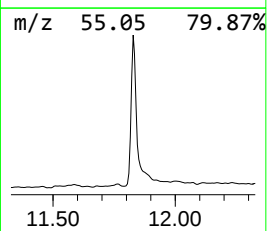
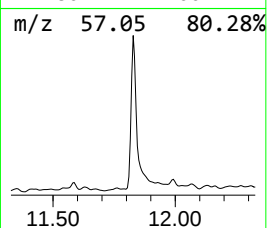
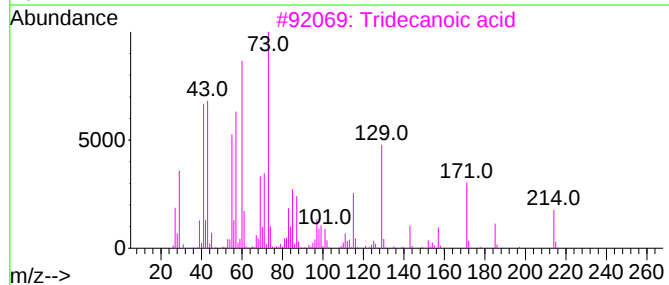
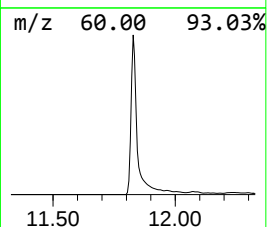
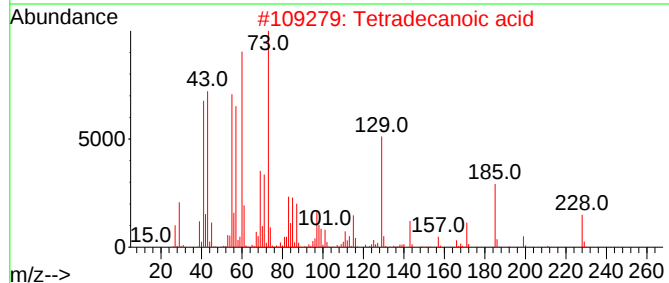
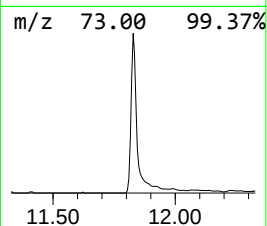
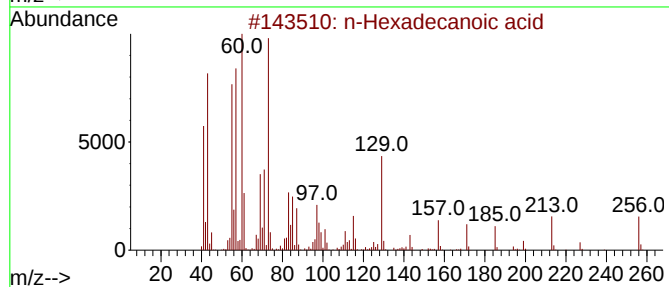
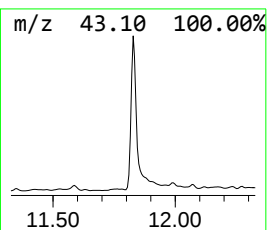
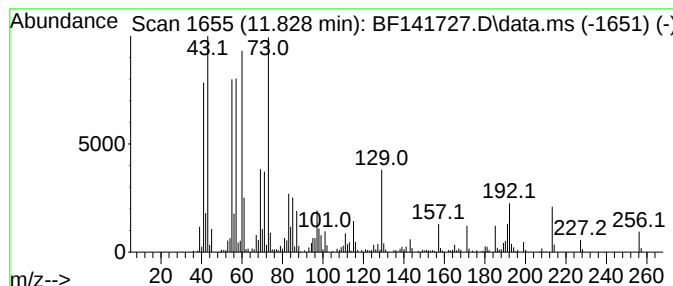
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.828	17.77 ng	567850	Phenanthrene-d10	11.298

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	93
3			Tridecanoic acid	214	C13H26O2	000638-53-9	91
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
5			n-Decanoic acid	172	C10H20O2	000334-48-5	60



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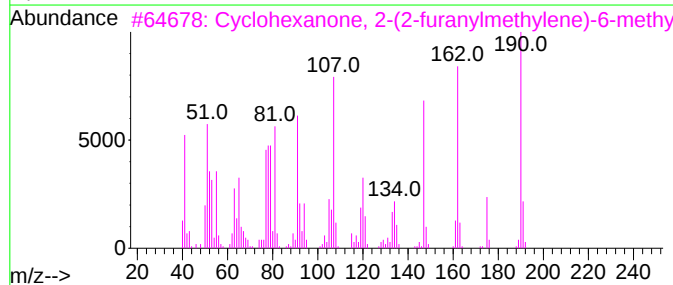
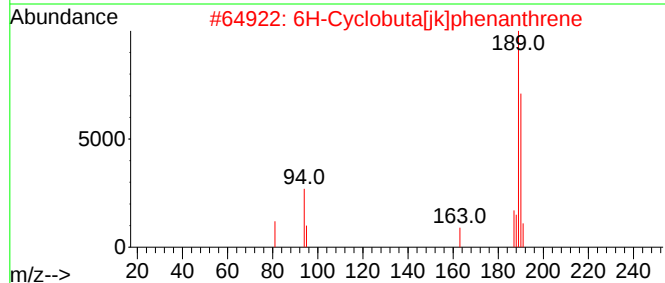
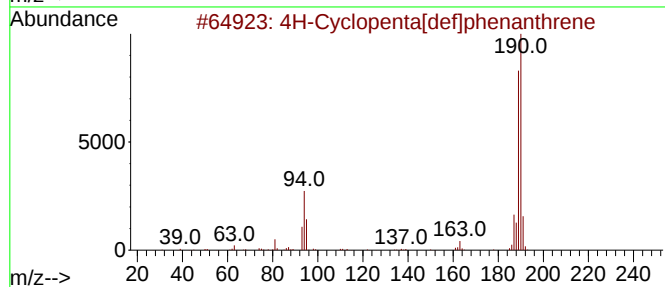
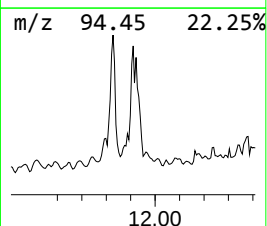
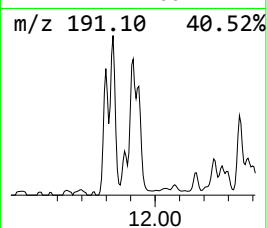
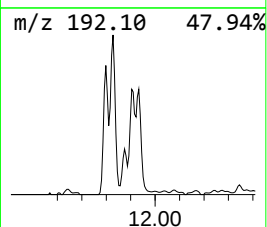
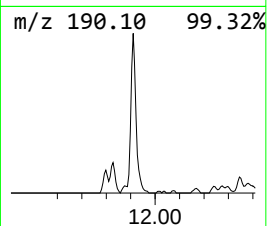
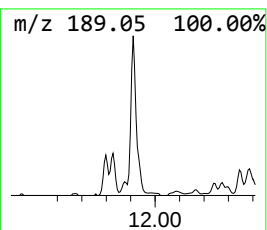
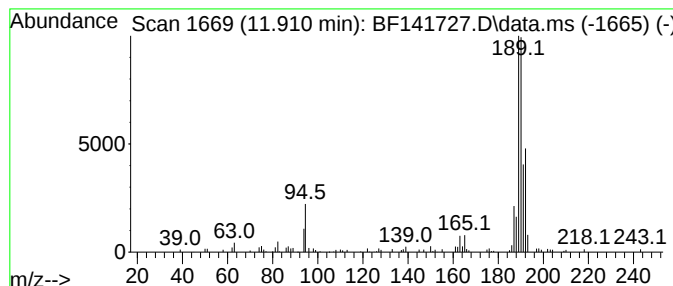
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.910	5.30 ng	169283	Phenanthrene-d10	11.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	76
2			6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	53
3			Cyclohexanone, 2-(2-furanylmethy...	190	C12H14O2	056053-07-7	27
4			2,4(1H,3H)-Pyrimidinedione, 5-br...	190	C4H3BrN2O2	000051-20-7	25
5			2-Amino-4,6-dichloropyrimidine-5...	191	C5H3Cl2N3O	005604-46-6	25



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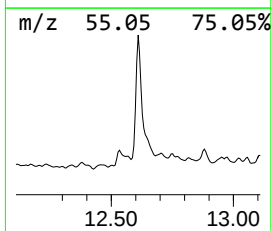
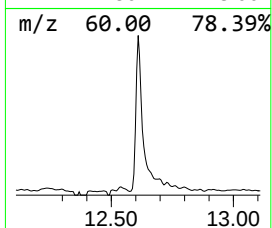
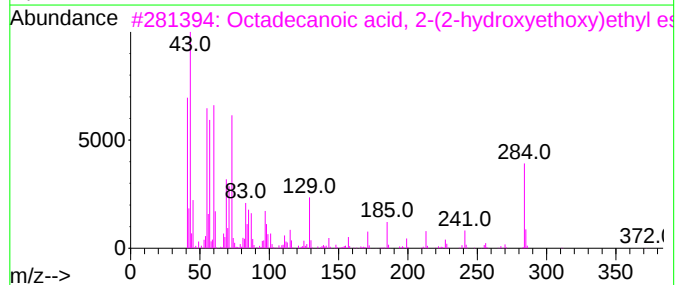
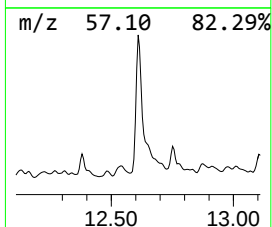
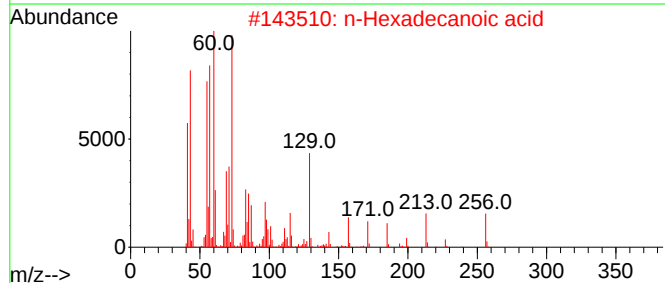
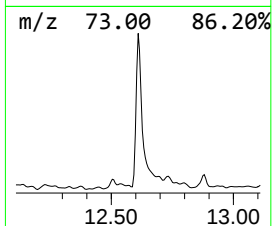
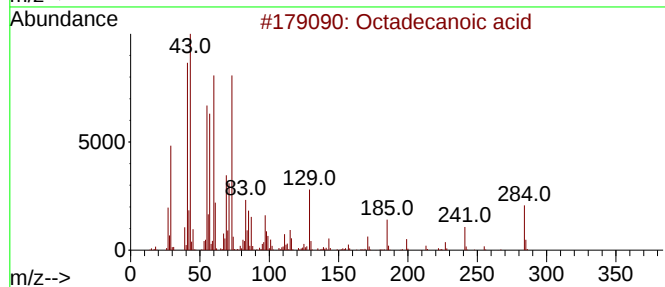
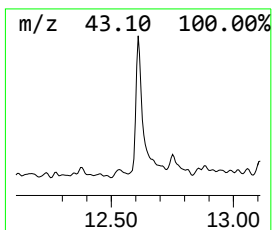
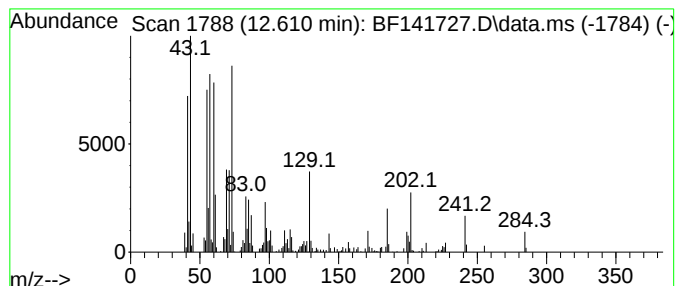
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.610	5.09 ng	162675	Phenanthrene-d10	11.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	76
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5			Undecanoic acid	186	C11H22O2	000112-37-8	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022125\
Data File : BF141727.D
Acq On : 21 Feb 2025 18:44
Operator : RC/JU
Sample : Q1397-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
STOCK-PILE

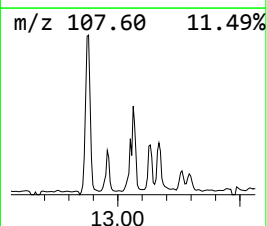
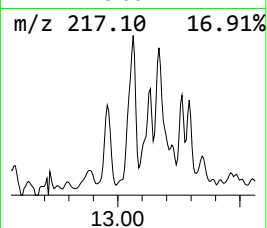
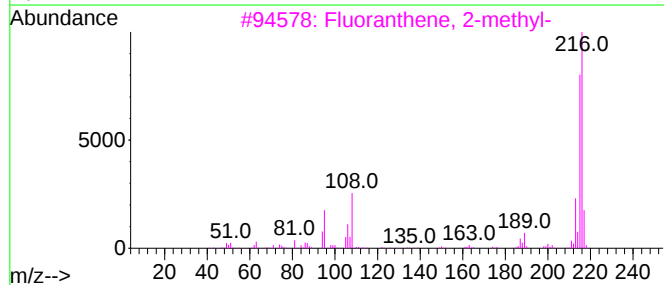
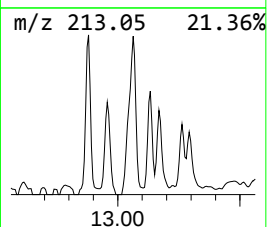
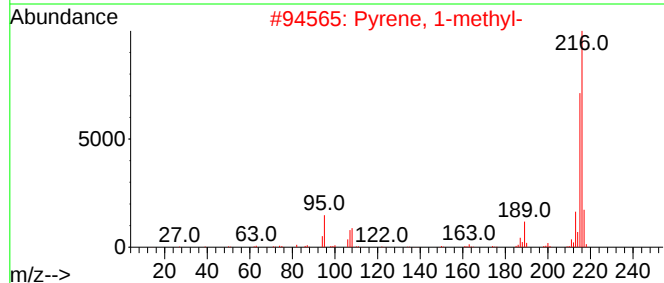
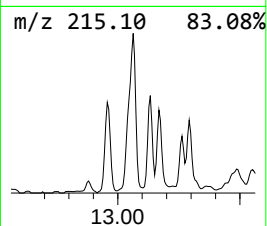
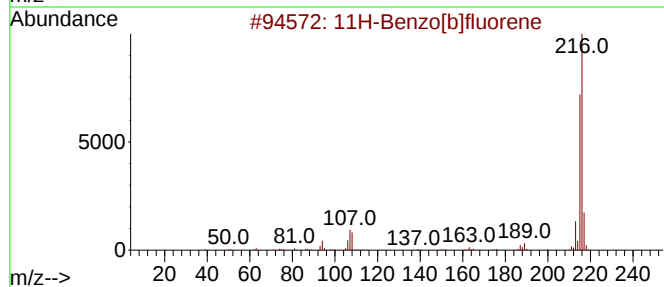
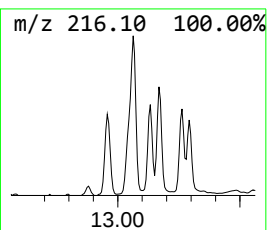
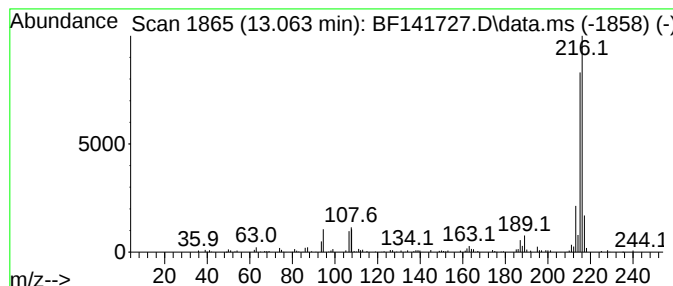
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 11H-Benzo[b]fluorene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.063	2.83 ng	150948	Chrysene-d12	13.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11H-Benzo[b]fluorene	216	C17H12	000243-17-4	94
2			Pyrene, 1-methyl-	216	C17H12	002381-21-7	94
3			Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	91
4			11H-Benzo[a]fluorene	216	C17H12	000238-84-6	91
5			7H-Benzo[c]fluorene	216	C17H12	000205-12-9	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022125\
Data File : BF141727.D
Acq On : 21 Feb 2025 18:44
Operator : RC/JU
Sample : Q1397-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

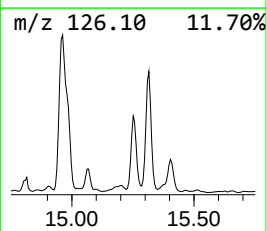
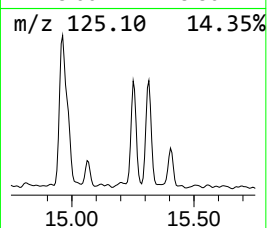
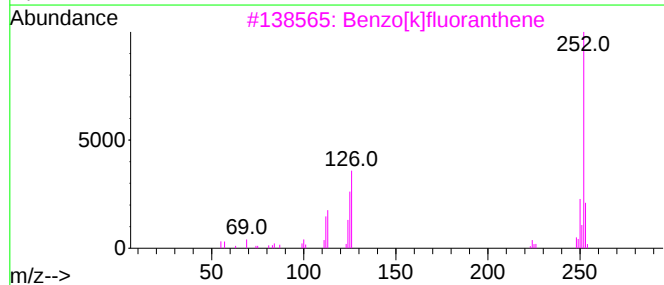
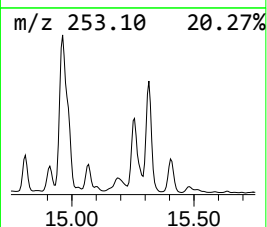
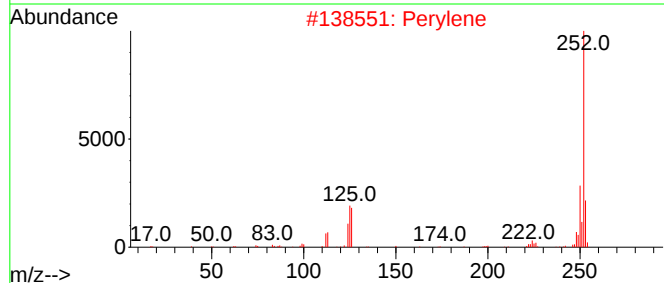
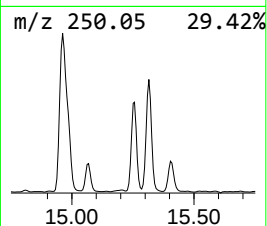
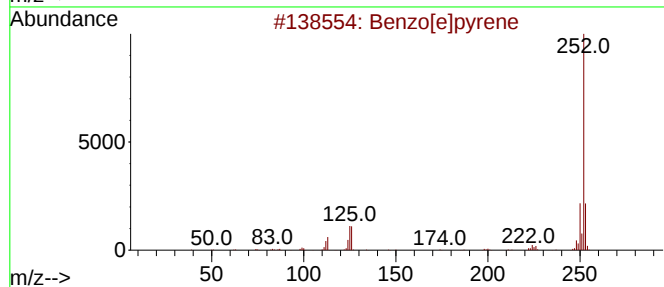
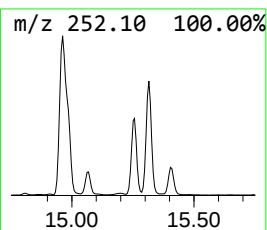
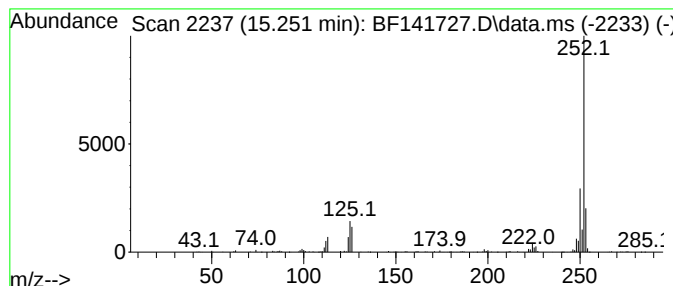
Instrument :
BNA_F
ClientSampleId :
STOCK-PILE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020625.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzo[e]pyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.251	7.70 ng	188865	Perylene-d12	15.374	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Perylene	252	C20H12	000198-55-0	96
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	94
5	Benzo[a]pyrene	252	C20H12	000050-32-8	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022125\
Data File : BF141727.D
Acq On : 21 Feb 2025 18:44
Operator : RC/JU
Sample : Q1397-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
STOCK-PILE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020625.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.987	2.6	ng	71933	1	6.781	551316	20.0
Benzophenone	10.522	5.4	ng	202340	3	9.810	750558	20.0
n-Hexadecanoic ...	11.828	17.8	ng	567850	4	11.298	639169	20.0
4H-Cyclopenta[d...]	11.910	5.3	ng	169283	4	11.298	639169	20.0
Octadecanoic acid	12.610	5.1	ng	162675	4	11.298	639169	20.0
11H-Benzo[b]flu...	13.063	2.8	ng	150948	5	13.933	1065760	20.0
Benzo[e]pyrene	15.251	7.7	ng	188865	6	15.374	490574	20.0