LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072225\
Data File : BF143206.D
Acq On : 22 Jul 2025 23:43
Operator : RC/JU
Sample : Q2649-17
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-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-BF071725.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF143206.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.304	12	19	29	rVB	543370	867654	51.49%	3.843%
2	5.198	504	511	517	rBV	145295	198887	11.80%	0.881%
3	5.604	574	580	585	rBV	1202317	1555170	92.29%	6.888%
4	6.598	743	749	754	rBV	1283268	1685118	100.00%	7.464%
5	6.969	807	812	817	rVB	546894	666182	39.53%	2.951%
6	7.522	898	906	911	rBV	806906	1018112	60.42%	4.510%
7	7.769	944	948	953	rVB	19678	23975	1.42%	0.106%
8	8.251	1024	1030	1038	rBV	626381	819635	48.64%	3.630%
9	8.457	1060	1065	1069	rVB	15132	19033	1.13%	0.084%
10	9.322	1207	1212	1217	rBV	1319665	1610792	95.59%	7.135%
11	9.669	1266	1271	1284	rBV2	179110	242558	14.39%	1.074%
12	9.863	1300	1304	1310	rBV2	15001	19041	1.13%	0.084%
13	10.004	1319	1328	1332	rBV	607501	871550	51.72%	3.860%
14	10.033	1332	1333	1340	rVB	19650	20700	1.23%	0.092%
15	10.204	1358	1362	1366	rBV2	26636	34694	2.06%	0.154%
16	10.410	1391	1397	1403	rBV	57663	88739	5.27%	0.393%
17	10.551	1417	1421	1426	rVB2	18876	24634	1.46%	0.109%
18	10.710	1441	1448	1457	rVB	227878	291515	17.30%	1.291%
19	10.792	1457	1462	1467	rBV	675646	840433	49.87%	3.723%
20	10.986	1491	1495	1498	rVV2	21316	27485	1.63%	0.122%
21	11.022	1498	1501	1505	rVB	26508	32087	1.90%	0.142%
22	11.074	1506	1510	1518	rBV4	23507	43452	2.58%	0.192%
23	11.151	1518	1523	1532	rBV	137434	195964	11.63%	0.868%
24	11.292	1544	1547	1552	rVB	13372	17739	1.05%	0.079%
25	11.351	1552	1557	1559	rBV4	11629	19172	1.14%	0.085%
26	11.386	1560	1563	1567	rVB	19155	25727	1.53%	0.114%
27	11.492	1574	1581	1590	rBV2	500119	869505	51.60%	3.851%
28	11.569	1590	1594	1595	rVV	52135	67088	3.98%	0.297%
29	11.592	1595	1598	1604	rVB2	55952	77291	4.59%	0.342%
30	11.716	1614	1619	1625	rBV2	26569	43397	2.58%	0.192%
31	11.780	1626	1630	1634	rBV4	26567	40150	2.38%	0.178%
32	11.863	1640	1644	1649	rVB6	15453	22304	1.32%	0.099%
33	11.939	1652	1657	1662	rBV	201735	291954	17.33%	1.293%
34	12.016	1664	1670	1677	rBV3	504862	741817	44.02%	3.286%
35	12.110	1682	1686	1693	rVB2	36144	78245	4.64%	0.347%
36	12.286	1713	1716	1722	rBV2	15396	30420	1.81%	0.135%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072225\
Data File : BF143206.D
Acq On : 22 Jul 2025 23:43
Operator : RC/JU
Sample : Q2649-17
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-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-BF071725.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.533	1754	1758	1763	rVB3	23985	40130	2.38%	0.178%
38	12.710	1782	1788	1799	rBV2	403554	1001436	59.43%	4.436%
39	12.798	1800	1803	1811	rVB2	71336	119017	7.06%	0.527%
40	12.933	1820	1826	1831	rVB	212302	301331	17.88%	1.335%
41	13.074	1845	1850	1857	rVB	1051653	1354905	80.40%	6.001%
42	13.151	1860	1863	1871	rVV3	30150	56777	3.37%	0.251%
43	13.327	1891	1893	1896	rBV2	29431	33935	2.01%	0.150%
44	13.363	1897	1899	1906	rVB2	41237	52273	3.10%	0.232%
45	13.833	1975	1979	1983	rVB	287209	339652	20.16%	1.504%
46	13.968	1998	2002	2009	rVB2	152821	225766	13.40%	1.000%
47	14.133	2023	2030	2033	rBV	701450	1257311	74.61%	5.569%
48	14.998	2172	2177	2185	rBV	957393	1383260	82.09%	6.127%
49	15.198	2206	2211	2220	rVB	560567	1243023	73.76%	5.506%
50	15.515	2261	2265	2271	rVB	356617	546284	32.42%	2.420%
51	15.580	2271	2276	2281	rBV	270523	407768	24.20%	1.806%
52	15.645	2282	2287	2291	rBV	416395	691438	41.03%	3.063%

Sum of corrected areas: 22576525

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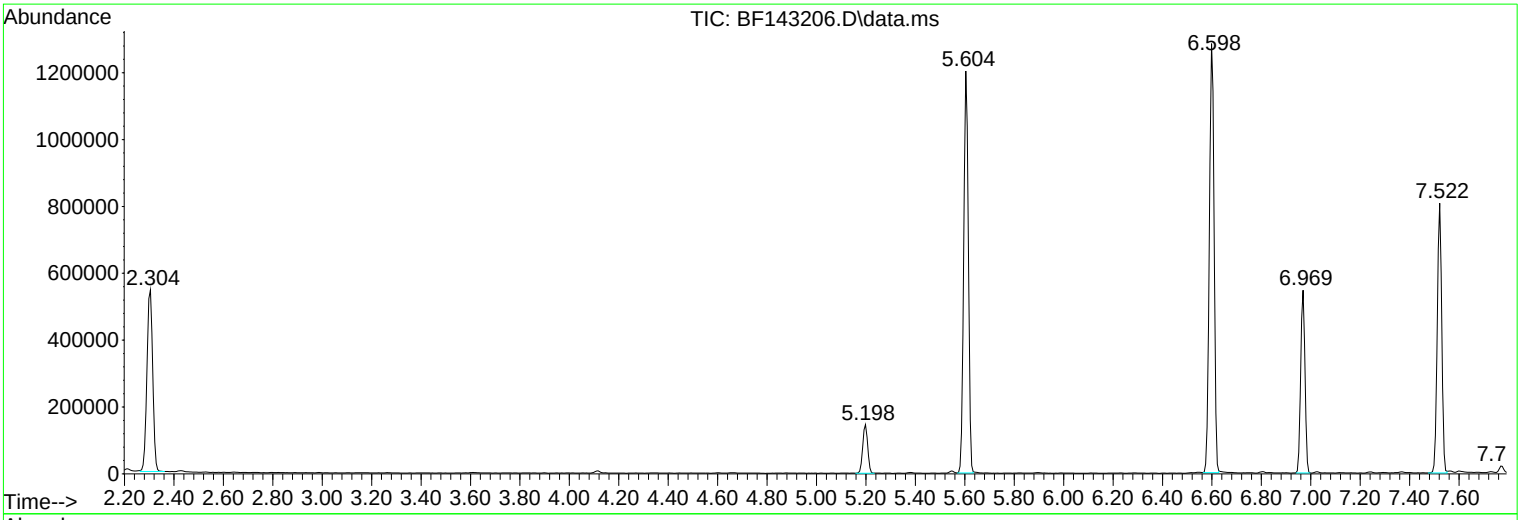
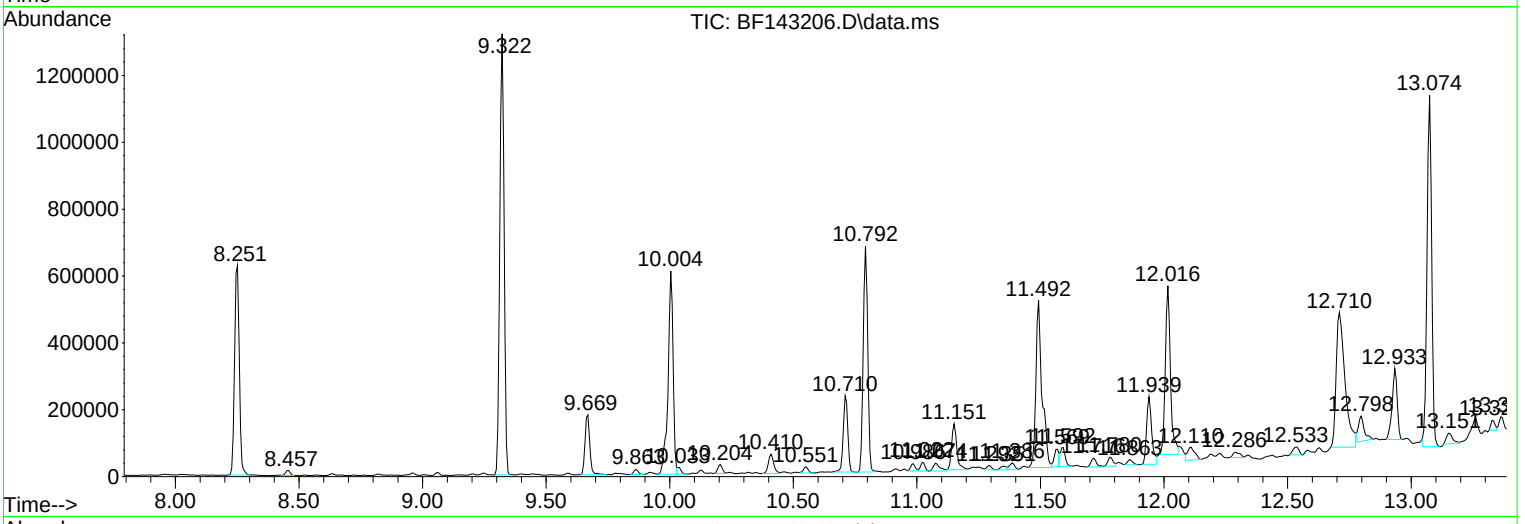
Misc :
ALS Vial : 19 Sample Multiplier: 1

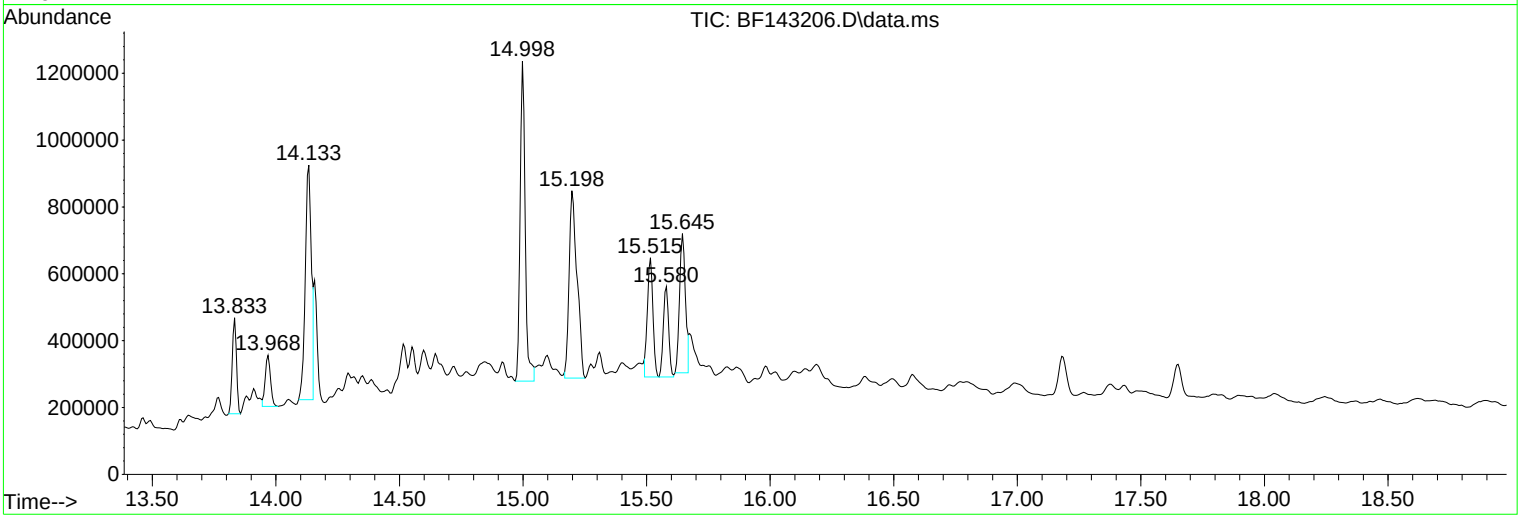
Instrument :
BNA_F
ClientSampleId :
WC-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071725.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 : BF143206.D
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Operator : RC/JU
Sample : Q2649-17
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071725.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

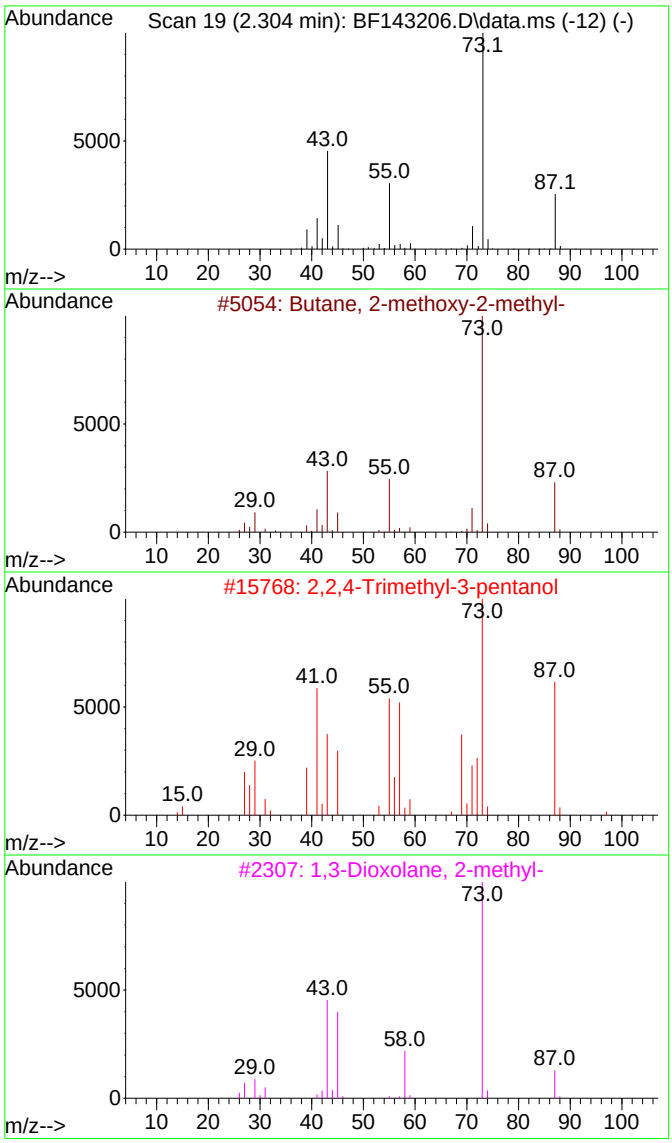
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

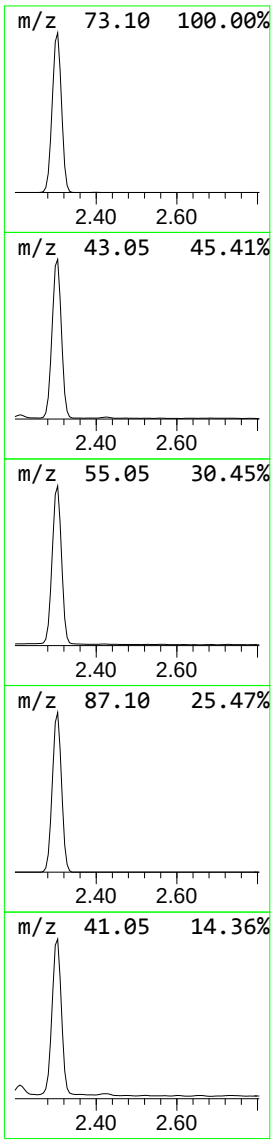
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.304	26.05 ng	867654	1,4-Dichlorobenzene-d4	6.969

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	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072225\
Data File : BF143206.D
Acq On : 22 Jul 2025 23:43
Operator : RC/JU
Sample : Q2649-17
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-5

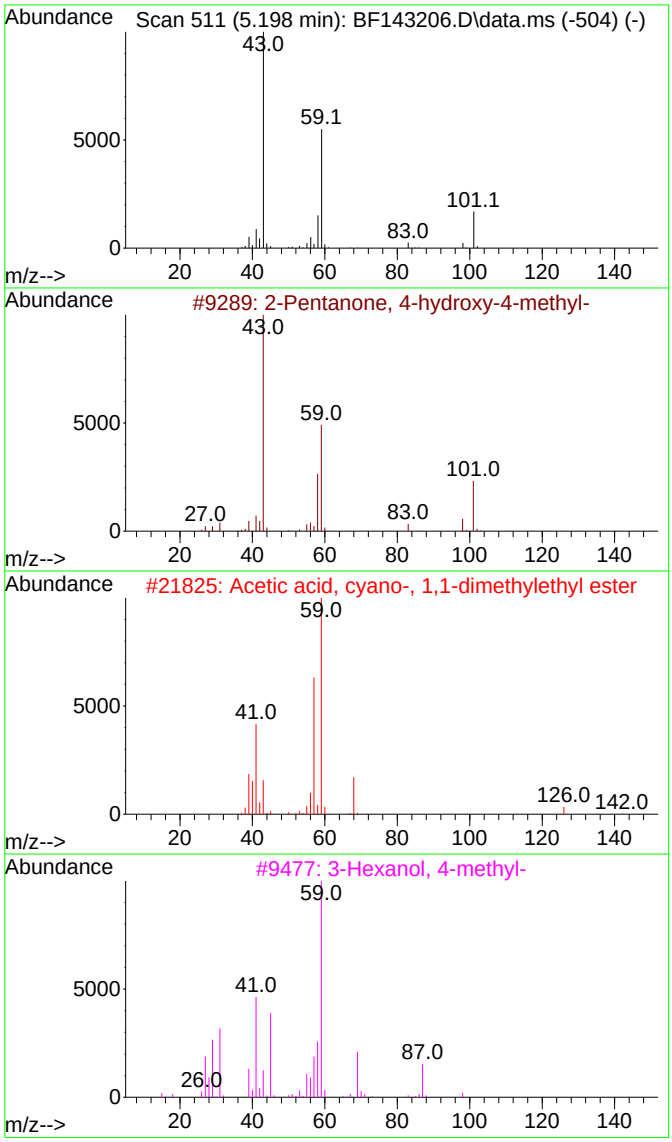
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071725.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

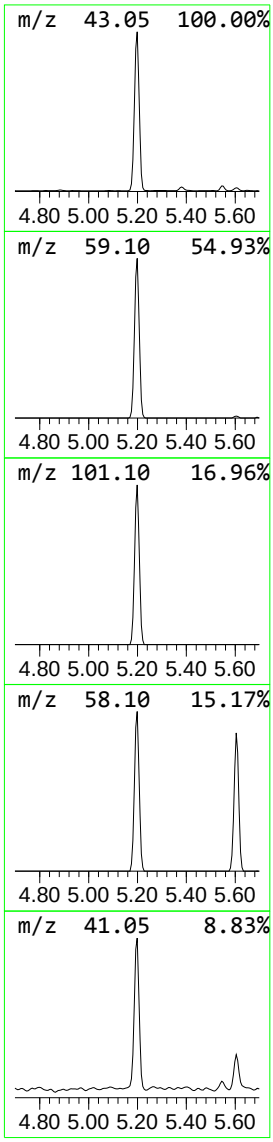
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.198	5.97 ng	198887	1,4-Dichlorobenzene-d4	6.969

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	37
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072225\
Data File : BF143206.D
Acq On : 22 Jul 2025 23:43
Operator : RC/JU
Sample : Q2649-17
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071725.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

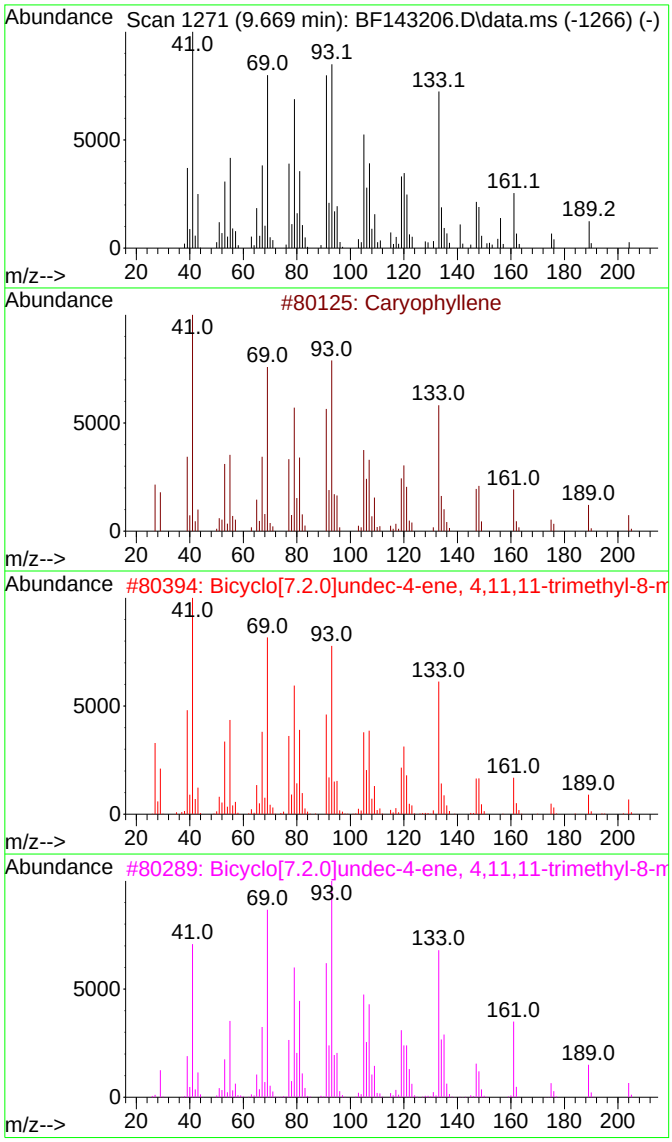
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

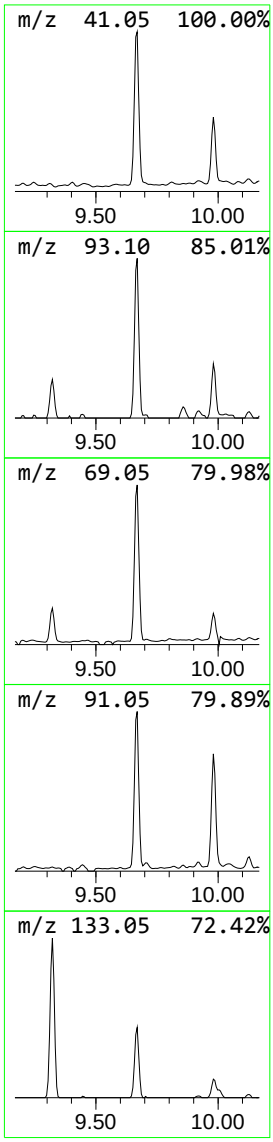
****

Peak Number 3 Caryophyllene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.669	5.57 ng	242558	Acenaphthene-d10	10.004

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Caryophyllene	204	C15H24	000087-44-5	94
2	Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	000118-65-0	91
3	Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	013877-93-5	80
4	Bicyclo[5.2.0]nonane, 2-methylen...	204	C15H24	242794-76-9	38
5	(Z,Z)-.alpha.-Farnesene	204	C15H24	1000293-03-1	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072225\
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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071725.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

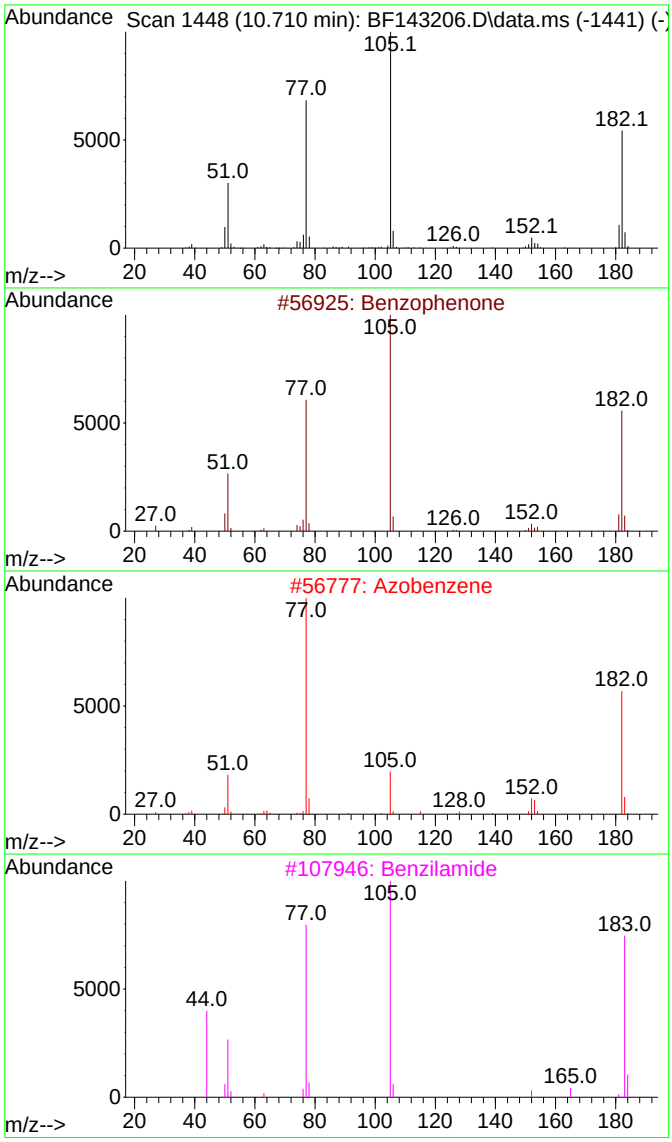
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

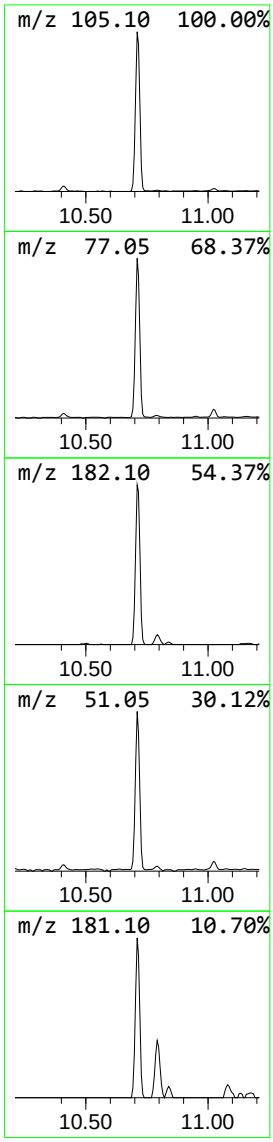
****

Peak Number 4 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.710	6.69 ng	291515	Acenaphthene-d10	10.004

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Azobenzene	182	C12H10N2	000103-33-3	52
3	Benzilamide	227	C14H13NO2	004746-87-6	50
4	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	50
5	Benzoylformic acid	150	C8H6O3	000611-73-4	49





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Data File : BF143206.D
Acq On : 22 Jul 2025 23:43
Operator : RC/JU
Sample : Q2649-17
Misc :
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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071725.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

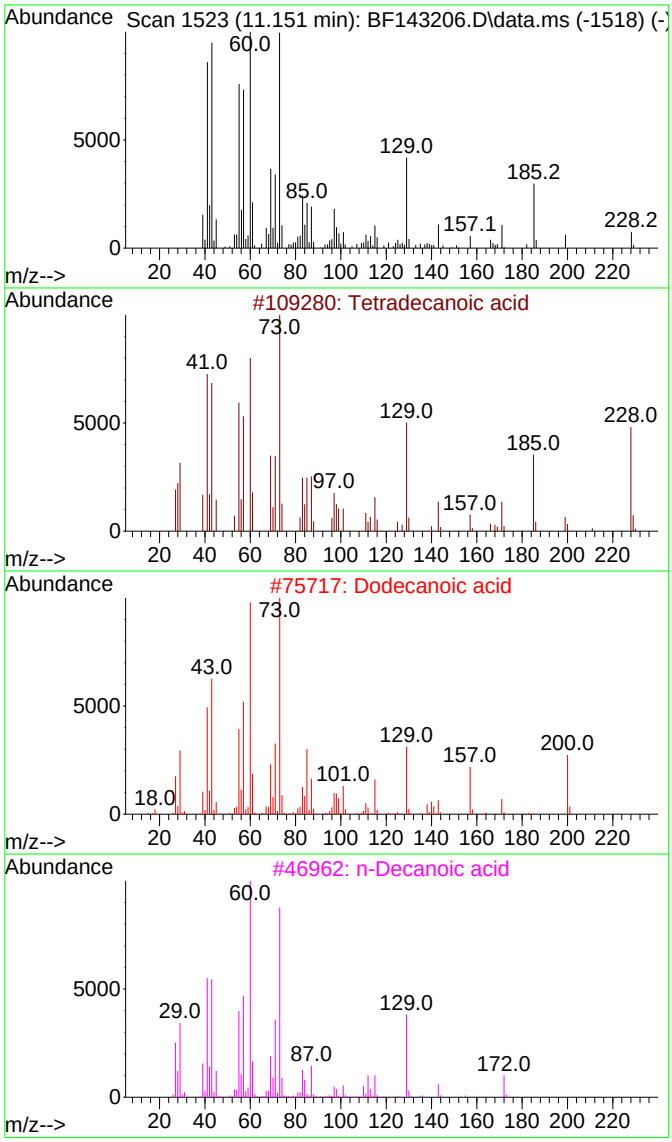
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

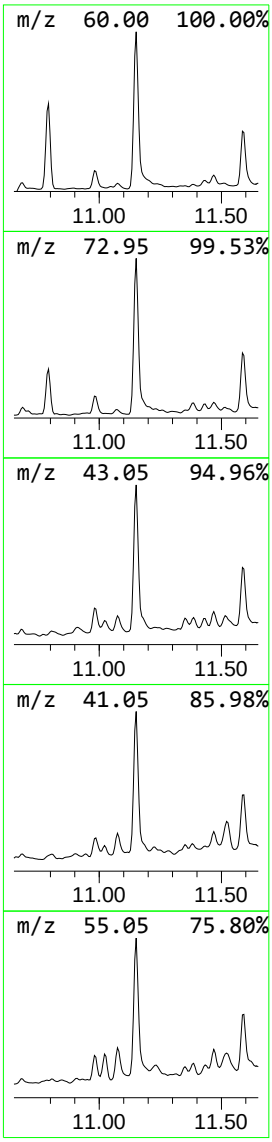
****

Peak Number 5 Tetradecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.151	4.51 ng	195964	Phenanthrene-d10	11.492

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
2	Dodecanoic acid	200	C12H24O2	000143-07-7	64
3	n-Decanoic acid	172	C10H20O2	000334-48-5	62
4	Tridecanoic acid	214	C13H26O2	000638-53-9	59
5	Undecanoic acid	186	C11H22O2	000112-37-8	58





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Operator : RC/JU
Sample : Q2649-17
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071725.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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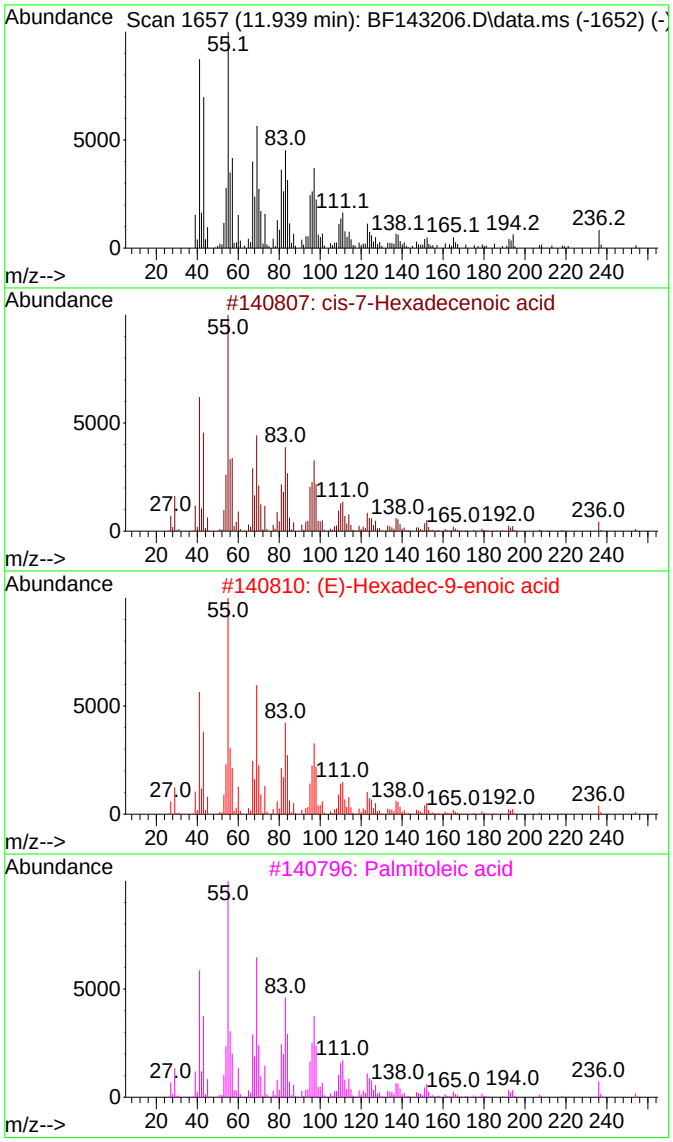
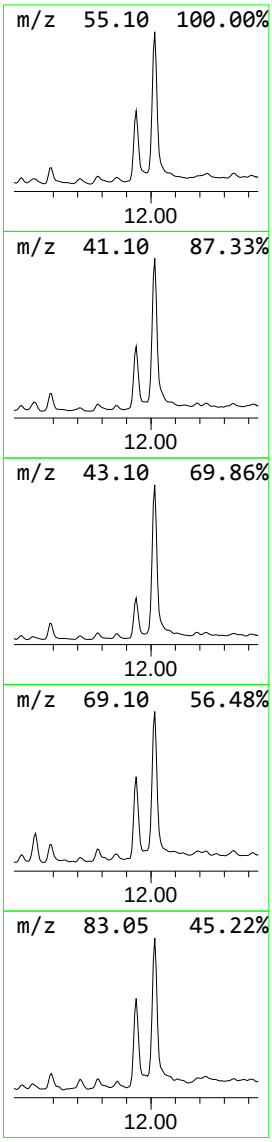
Peak Number 6 cis-7-Hexadecenoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.939	6.72 ng	291954	Phenanthrene-d10	11.492

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-7-Hexadecenoic acid	254	C16H30O2	002416-19-5	99
2	(E)-Hexadec-9-enoic acid	254	C16H30O2	010030-73-6	99
3	Palmitoleic acid	254	C16H30O2	000373-49-9	98
4	9-Hexadecenoic acid	254	C16H30O2	002091-29-4	93
5	Hexadecenoic acid, Z-11-	254	C16H30O2	002416-20-8	91





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Data File : BF143206.D
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Operator : RC/JU
Sample : Q2649-17
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071725.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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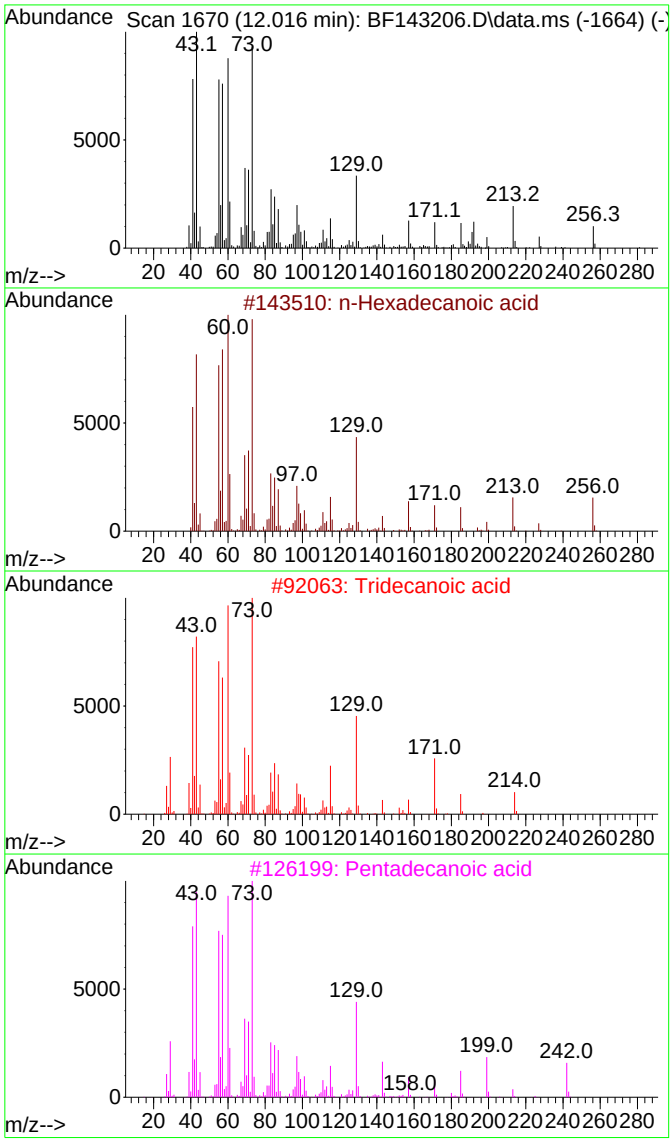
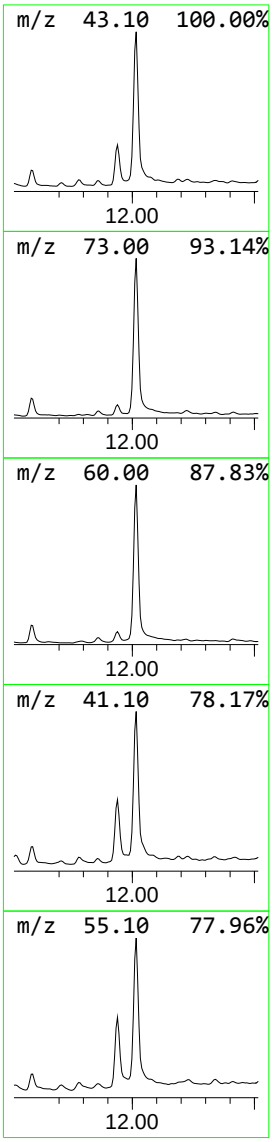
Peak Number 7 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.016	17.06 ng	741817	Phenanthrene-d10	11.492

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	62
5	Undecanoic acid	186	C11H22O2	000112-37-8	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072225\
Data File : BF143206.D
Acq On : 22 Jul 2025 23:43
Operator : RC/JU
Sample : Q2649-17
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071725.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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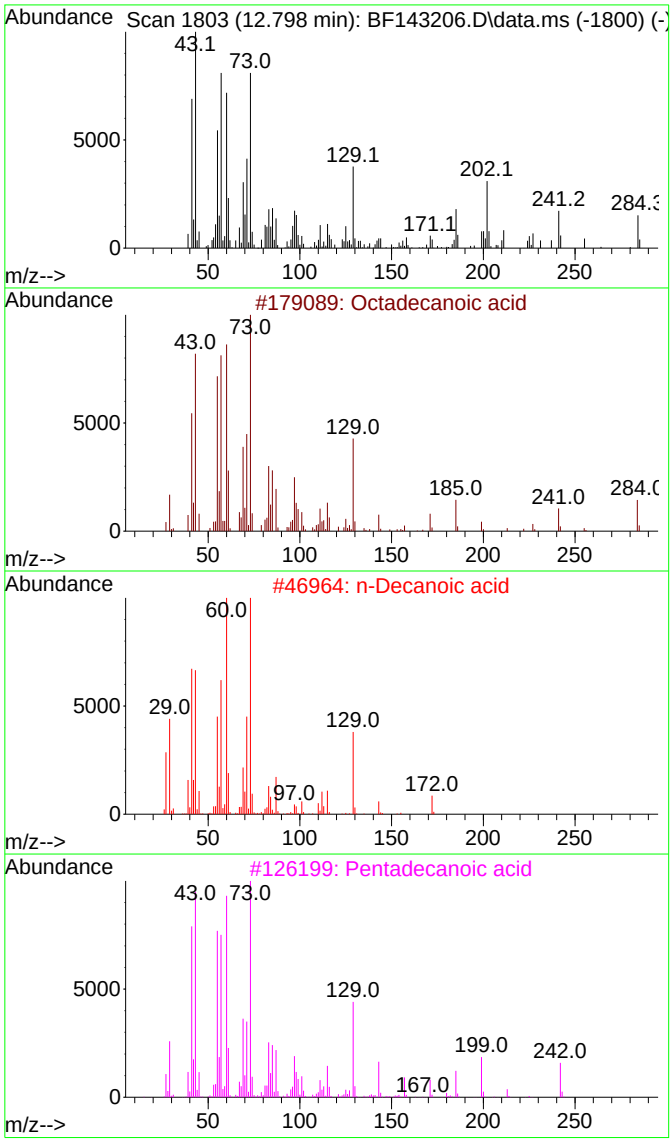
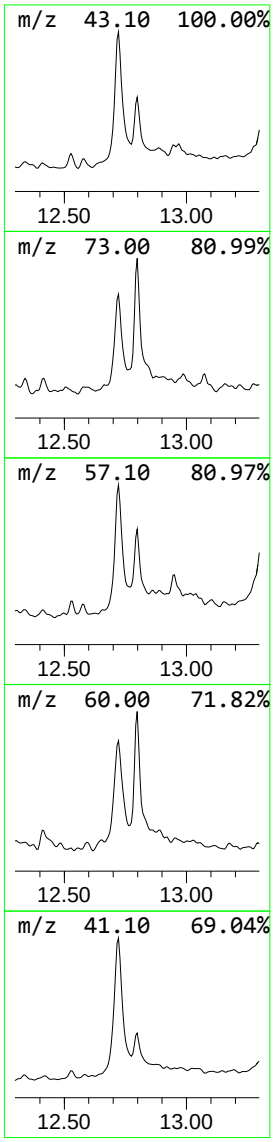
Peak Number 8 Octadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.798	2.74 ng	119017	Phenanthrene-d10	11.492

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	n-Decanoic acid	172	C10H20O2	000334-48-5	64
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	55
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	50
5	Dodecanoic acid	200	C12H24O2	000143-07-7	43





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Data File : BF143206.D
Acq On : 22 Jul 2025 23:43
Operator : RC/JU
Sample : Q2649-17
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071725.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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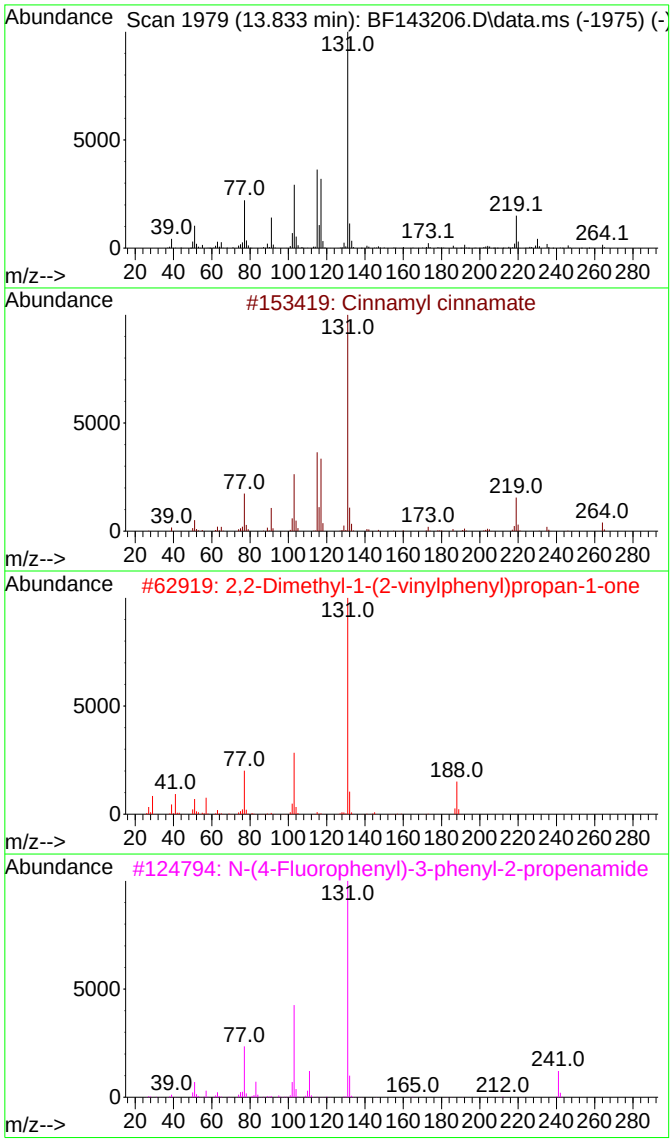
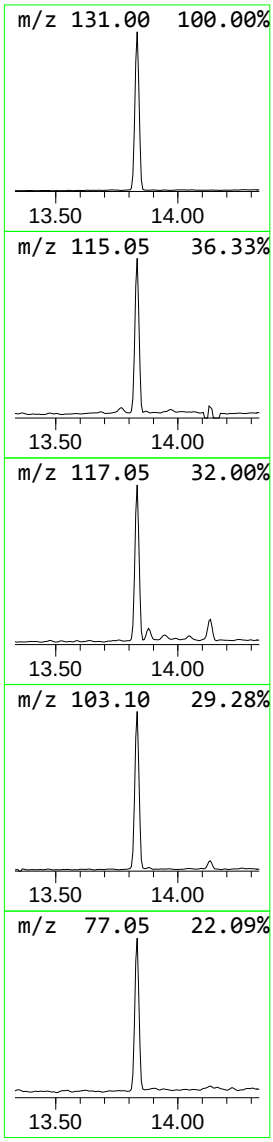
Peak Number 9 Cinnamyl cinnamate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.833	5.40 ng	339652	Chrysene-d12	14.133

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cinnamyl cinnamate	264	C18H16O2	000122-69-0	91
2	2,2-Dimethyl-1-(2-vinylphenyl)pr...	188	C13H16O	1000210-99-9	52
3	N-(4-Fluorophenyl)-3-phenyl-2-pr...	241	C15H12FNO	019358-27-1	50
4	p-Vinylbenzohydrazide	162	C9H10N2O	1000244-74-9	50
5	N-(p-Vinylbenzoyl)-l-alanine	219	C12H13NO3	139184-60-4	50





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Operator : RC/JU
Sample : Q2649-17
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071725.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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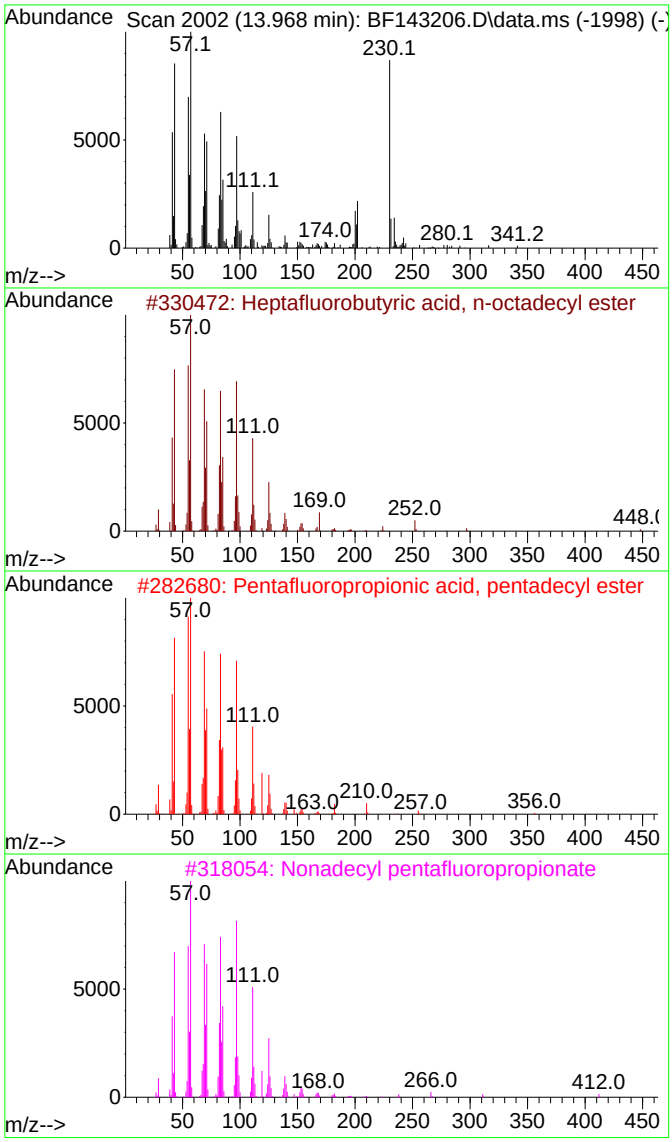
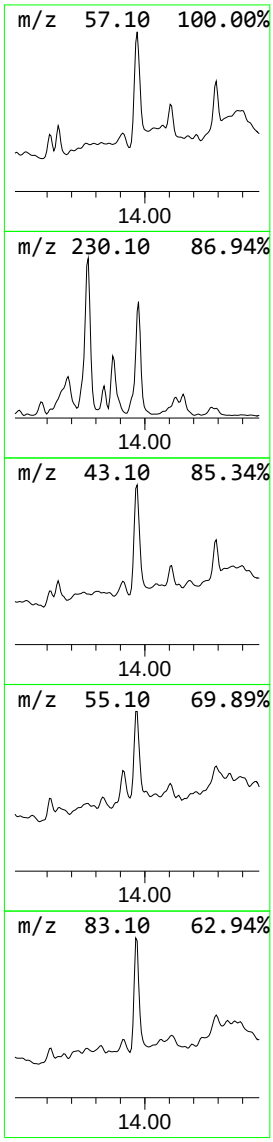
Peak Number 10 Heptafluorobutyric acid, n-... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.968	3.59 ng	225766	Chrysene-d12	14.133

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	60
2	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	60
3	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	60
4	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	60
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	60





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Data File : BF143206.D
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Operator : RC/JU
Sample : Q2649-17
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071725.M
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TIC Library : C:\Database\NIST20.L
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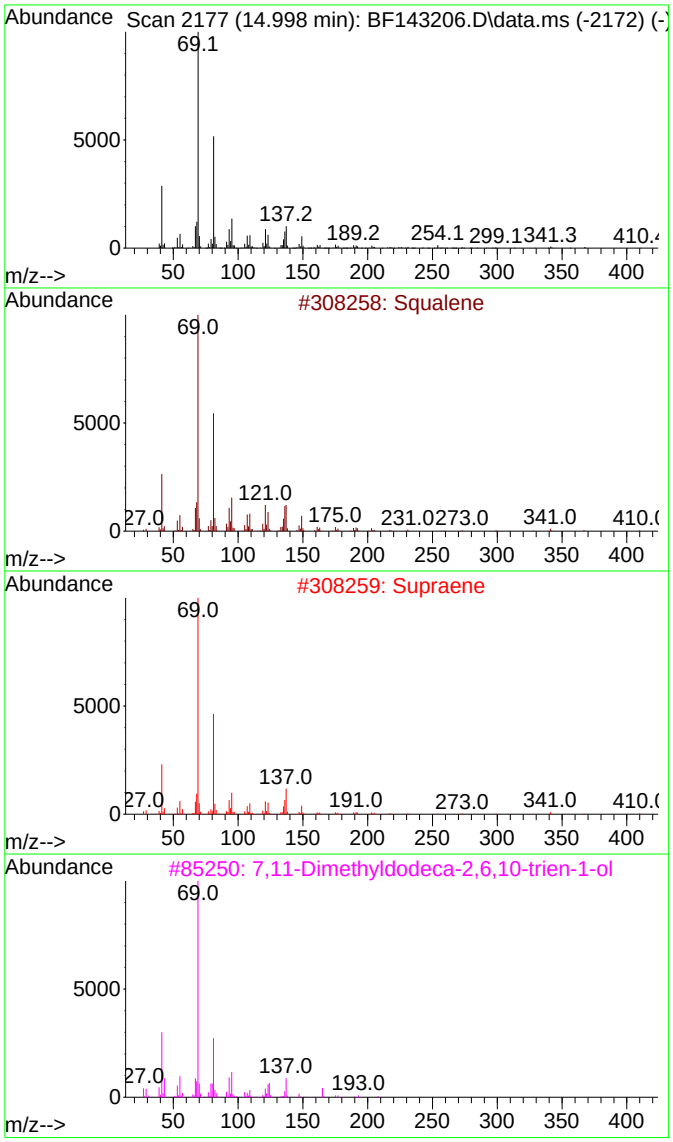
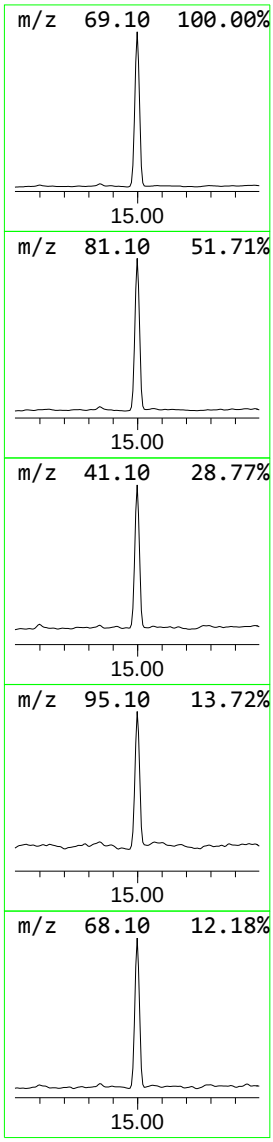
Peak Number 11 Squalene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.998	40.01 ng	1383260	Perylene-d12	15.645

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	94
2	Supraene	410	C30H50	007683-64-9	91
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	64
5	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	52





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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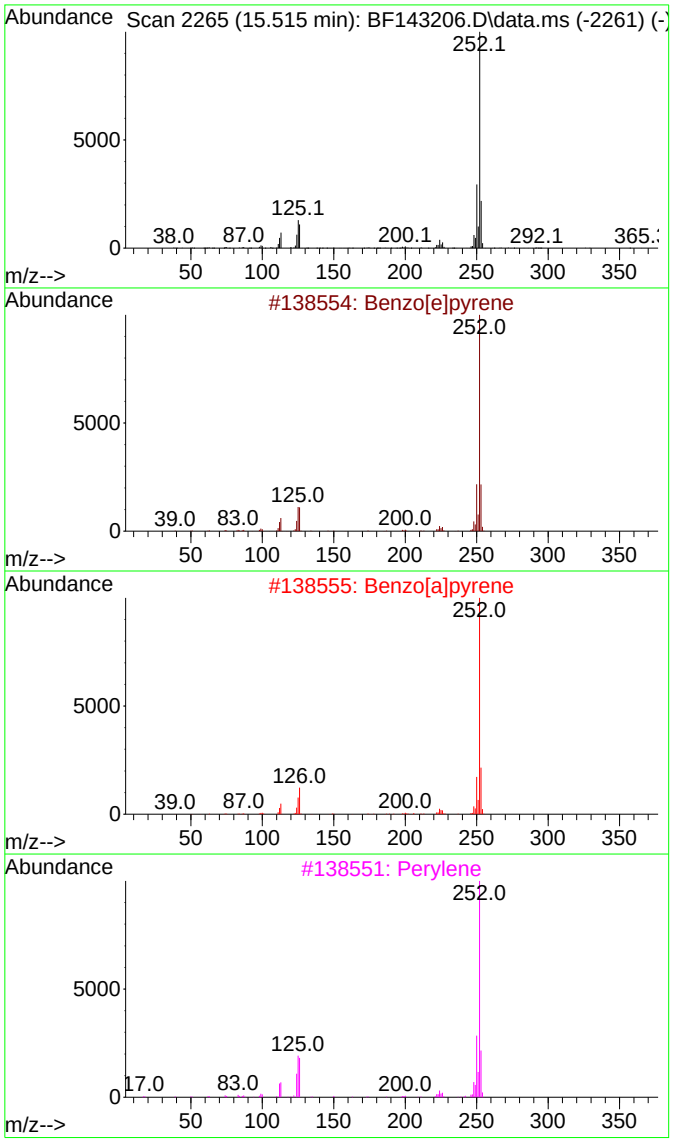
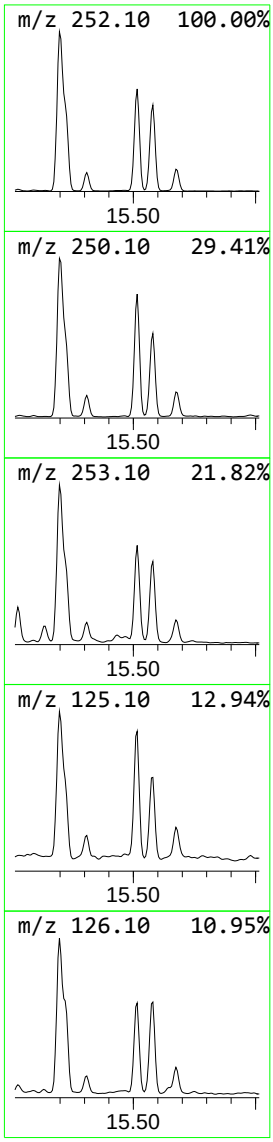
Peak Number 12 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.515	15.80 ng	546284	Perylene-d12	15.645

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	99
2	Benzo[a]pyrene	252	C20H12	000050-32-8	98
3	Perylene	252	C20H12	000198-55-0	97
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
5	Benzo[b]fluoranthene	252	C20H12	000205-99-2	94





Tentatively Identified Compound (LSC) summary

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Data File : BF143206.D
Acq On : 22 Jul 2025 23:43
Operator : RC/JU
Sample : Q2649-17
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071725.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...	2.304	26.1	ng	867654	1	6.969	666182	20.0
2-Pentanone, 4-...	5.198	6.0	ng	198887	1	6.969	666182	20.0
Caryophyllene	9.669	5.6	ng	242558	3	10.004	871550	20.0
Benzophenone	10.710	6.7	ng	291515	3	10.004	871550	20.0
Tetradecanoic acid	11.151	4.5	ng	195964	4	11.492	869505	20.0
cis-7-Hexadecen...	11.939	6.7	ng	291954	4	11.492	869505	20.0
n-Hexadecanoic ...	12.016	17.1	ng	741817	4	11.492	869505	20.0
Octadecanoic acid	12.798	2.7	ng	119017	4	11.492	869505	20.0
Cinnamyl cinnamate	13.833	5.4	ng	339652	5	14.133	1257310	20.0
Heptafluorobuty...	13.968	3.6	ng	225766	5	14.133	1257310	20.0
Squalene	14.998	40.0	ng	1383260	6	15.645	691438	20.0
Benzo[e]pyrene	15.515	15.8	ng	546284	6	15.645	691438	20.0