LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062723\
Data File : BF133998.D
Acq On : 27 Jun 2023 19:03
Operator : CG\JU
Sample : 03402-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP1-0623

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-BF062623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133998.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	8	14	19	rBV	1076685	1418280	64.65%	7.249%
2	2.281	29	33	41	rVB	38651	54768	2.50%	0.280%
3	3.969	317	320	325	rVB	27769	35152	1.60%	0.180%
4	5.093	506	511	523	rVB	74615	108532	4.95%	0.555%
5	5.451	569	572	574	rBV	37591	37121	1.69%	0.190%
6	5.487	574	578	581	rVV	2274527	2025505	92.33%	10.353%
7	5.704	612	615	619	rBV	36714	34415	1.57%	0.176%
8	6.487	744	748	751	rBV	2126554	2038039	92.90%	10.417%
9	6.675	777	780	784	rBV2	45545	52636	2.40%	0.269%
10	6.851	806	810	813	rBV	867131	679459	30.97%	3.473%
11	7.410	901	905	908	rBV	1456842	1289478	58.78%	6.591%
12	7.439	908	910	914	rVB	55077	45757	2.09%	0.234%
13	8.128	1024	1027	1030	rBV	922360	750816	34.23%	3.838%
14	8.151	1030	1031	1034	rVB	84204	44435	2.03%	0.227%
15	8.545	1094	1098	1101	rBV	24422	26578	1.21%	0.136%
16	8.716	1124	1127	1132	rBV	57310	51470	2.35%	0.263%
17	8.845	1146	1149	1152	rVB	89297	75616	3.45%	0.387%
18	8.939	1162	1165	1169	rBV	62378	52787	2.41%	0.270%
19	9.204	1207	1210	1214	rBV	2424013	2193706	100.00%	11.213%
20	9.286	1220	1224	1226	rBV	61609	52833	2.41%	0.270%
21	9.475	1251	1256	1260	rBV2	34835	44719	2.04%	0.229%
22	9.545	1265	1268	1270	rBV	54568	52034	2.37%	0.266%
23	9.569	1270	1272	1275	rVB	34235	29152	1.33%	0.149%
24	9.639	1281	1284	1286	rBV	107949	80284	3.66%	0.410%
25	9.663	1286	1288	1293	rVB	34266	28206	1.29%	0.144%
26	9.745	1300	1302	1305	rBV	45699	41492	1.89%	0.212%
27	9.816	1312	1314	1316	rBV	52644	34081	1.55%	0.174%
28	9.886	1319	1326	1330	rBV	901168	794615	36.22%	4.062%
29	9.928	1330	1333	1336	rVB2	32066	37227	1.70%	0.190%
30	10.045	1348	1353	1355	rBV6	15633	23577	1.07%	0.121%
31	10.092	1357	1361	1364	rVB	47796	48366	2.20%	0.247%
32	10.298	1392	1396	1397	rBV2	27611	32107	1.46%	0.164%
33	10.316	1397	1399	1402	rVB	47294	40310	1.84%	0.206%
34	10.433	1416	1419	1426	rVB4	32563	44020	2.01%	0.225%
35	10.539	1433	1437	1443	rVB4	16853	23970	1.09%	0.123%
36	10.604	1443	1448	1451	rBV	198326	167519	7.64%	0.856%

LSC Area Percent Report

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Sample : 03402-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1-0623

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-BF062623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	10.680	1457	1461	1467	rBV	1375427	1144865	52.19%	5.852%
38	10.792	1477	1480	1481	rBV2	78749	66376	3.03%	0.339%
39	11.122	1532	1536	1538	rBV3	21357	26190	1.19%	0.134%
40	11.245	1554	1557	1560	rVB	28804	24044	1.10%	0.123%
41	11.275	1560	1562	1567	rVB	28646	29146	1.33%	0.149%
42	11.380	1576	1580	1583	rBV	786262	687584	31.34%	3.515%
43	11.404	1583	1584	1588	rVV	207140	140044	6.38%	0.716%
44	11.457	1590	1593	1596	rVV	39364	37989	1.73%	0.194%
45	11.486	1596	1598	1602	rVB3	31471	31645	1.44%	0.162%
46	11.674	1627	1630	1634	rVV2	28859	25982	1.18%	0.133%
47	11.716	1635	1637	1642	rVB4	20451	24619	1.12%	0.126%
48	11.886	1663	1666	1668	rBV	38595	37032	1.69%	0.189%
49	11.910	1668	1670	1675	rVB2	258028	227869	10.39%	1.165%
50	11.998	1682	1685	1687	rBV2	62305	62569	2.85%	0.320%
51	12.022	1687	1689	1693	rVB	33161	32715	1.49%	0.167%
52	12.439	1757	1760	1763	rBV	45272	49942	2.28%	0.255%
53	12.474	1763	1766	1768	rVV3	40651	40119	1.83%	0.205%
54	12.527	1772	1775	1779	rVB3	43558	51376	2.34%	0.263%
55	12.604	1784	1788	1791	rBV	269437	253038	11.53%	1.293%
56	12.704	1801	1805	1808	rBV3	70123	79562	3.63%	0.407%
57	12.833	1822	1827	1833	rBV	291650	297566	13.56%	1.521%
58	12.980	1848	1852	1855	rBV	1796351	1574258	71.76%	8.047%
59	13.674	1968	1970	1975	rVB	36528	33557	1.53%	0.172%
60	13.886	2003	2006	2013	rBV	162171	194962	8.89%	0.997%
61	14.039	2027	2032	2035	rBV2	578976	643995	29.36%	3.292%
62	14.063	2035	2036	2043	rVB	120824	114864	5.24%	0.587%
63	14.204	2058	2060	2063	rBV	45970	40477	1.85%	0.207%
64	14.515	2110	2113	2118	rBV2	75645	108368	4.94%	0.554%
65	15.104	2209	2213	2216	rBV	135704	221091	10.08%	1.130%
66	15.180	2224	2226	2230	rVB	73488	84280	3.84%	0.431%
67	15.415	2264	2266	2273	rVB	92360	109136	4.97%	0.558%
68	15.480	2274	2277	2284	rVB	101738	131184	5.98%	0.671%
69	15.545	2284	2288	2292	rBV	256899	348449	15.88%	1.781%

Sum of corrected areas: 19563955

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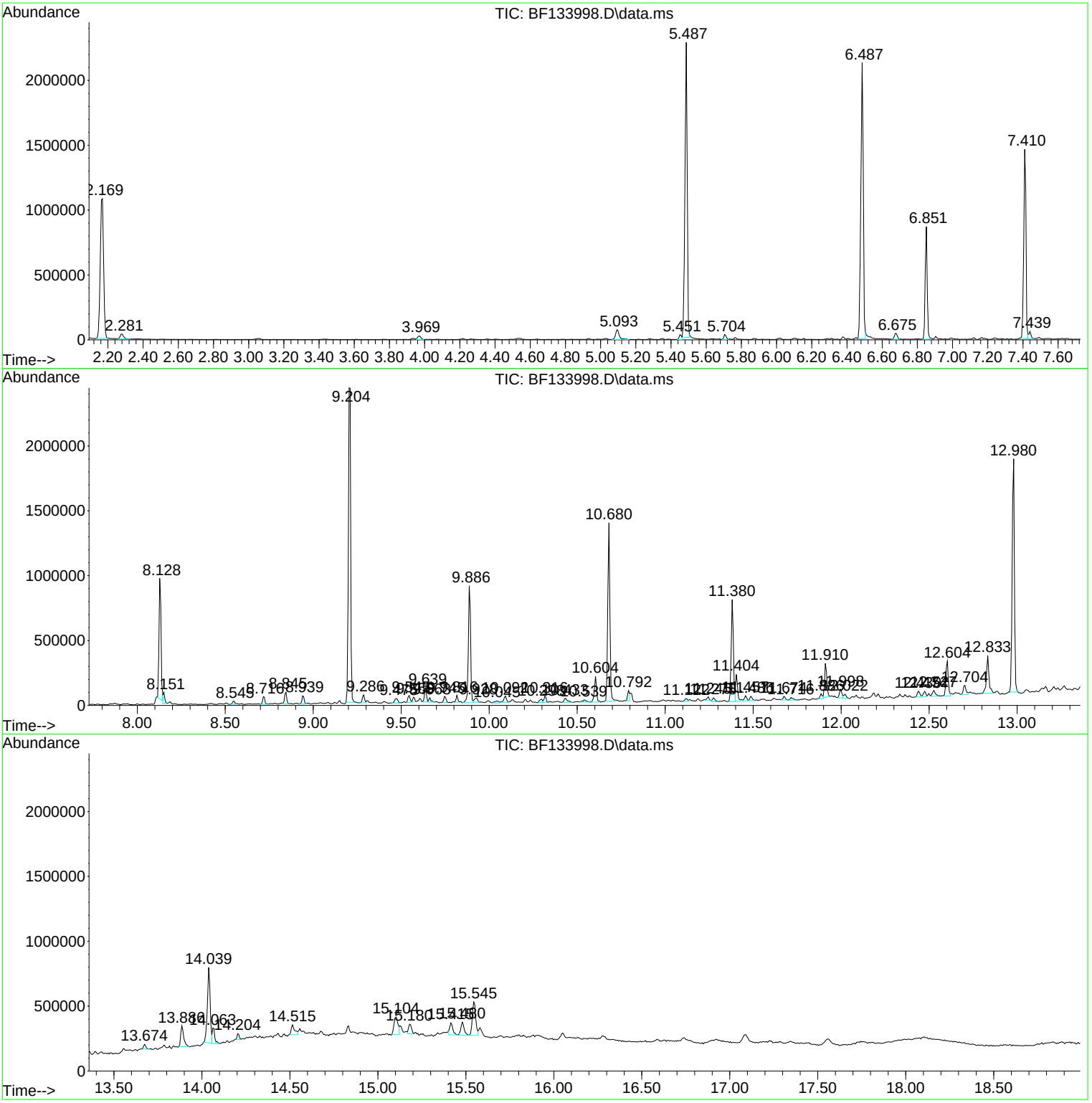
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1-0623

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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\BF062723\
Data File : BF133998.D
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

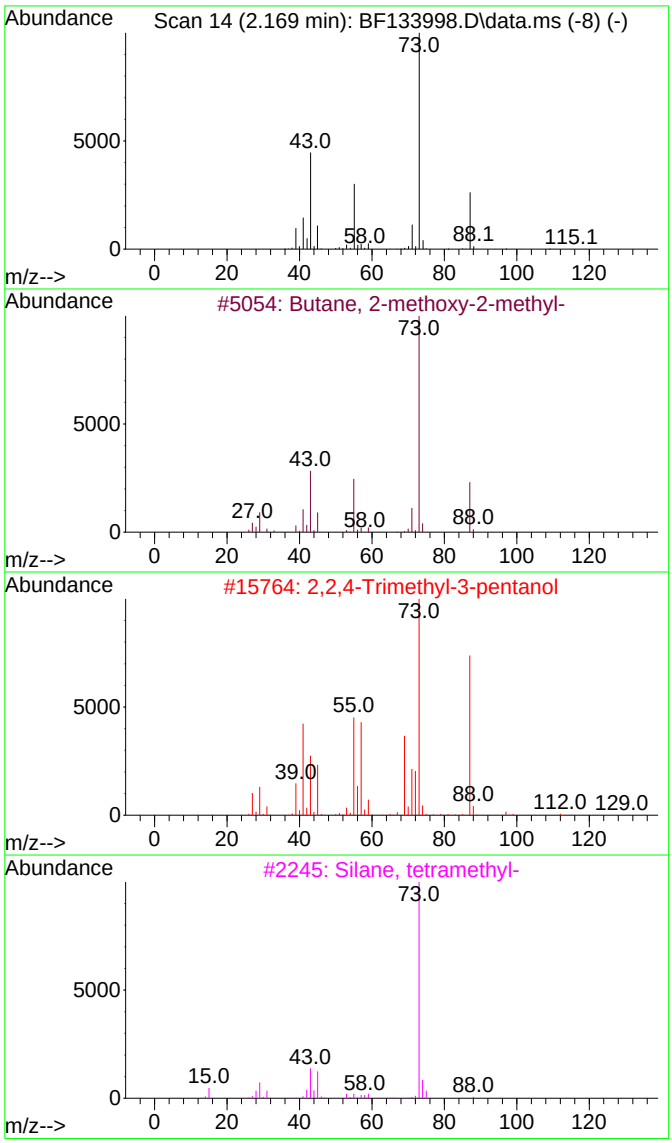
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

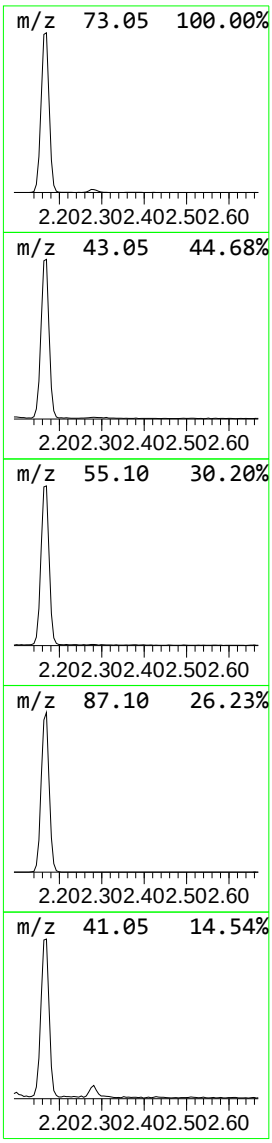
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.169	41.75 ng	1418280	1,4-Dichlorobenzene-d4	6.851

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	Silane, tetramethyl-	88	C4H12Si	000075-76-3	32
4	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062723\
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Acq On : 27 Jun 2023 19:03
Operator : CG\JU
Sample : 03402-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1-0623

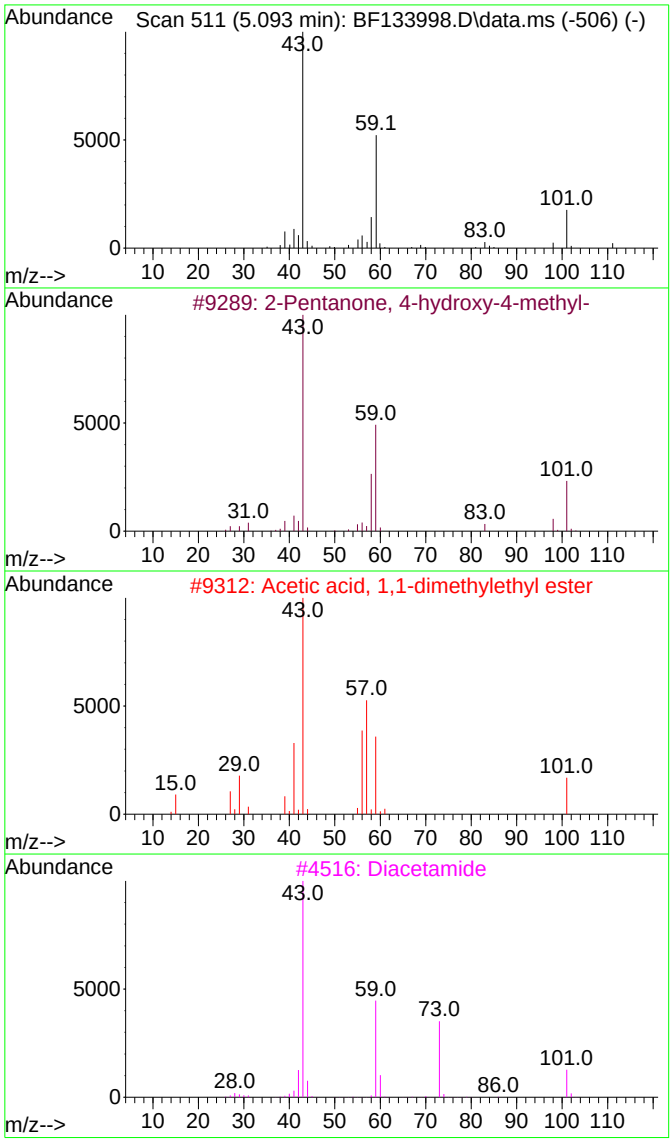
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

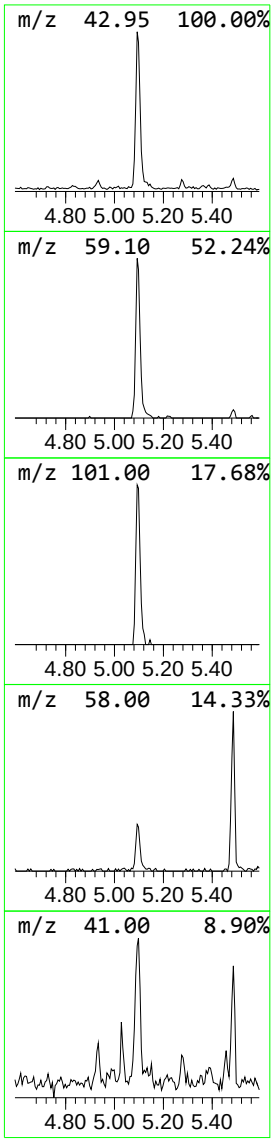
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.093	3.19 ng	108532	1,4-Dichlorobenzene-d4	6.851

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	Diacetamide	101	C4H7NO2	000625-77-4	36
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062723\
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Sample : 03402-01
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BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

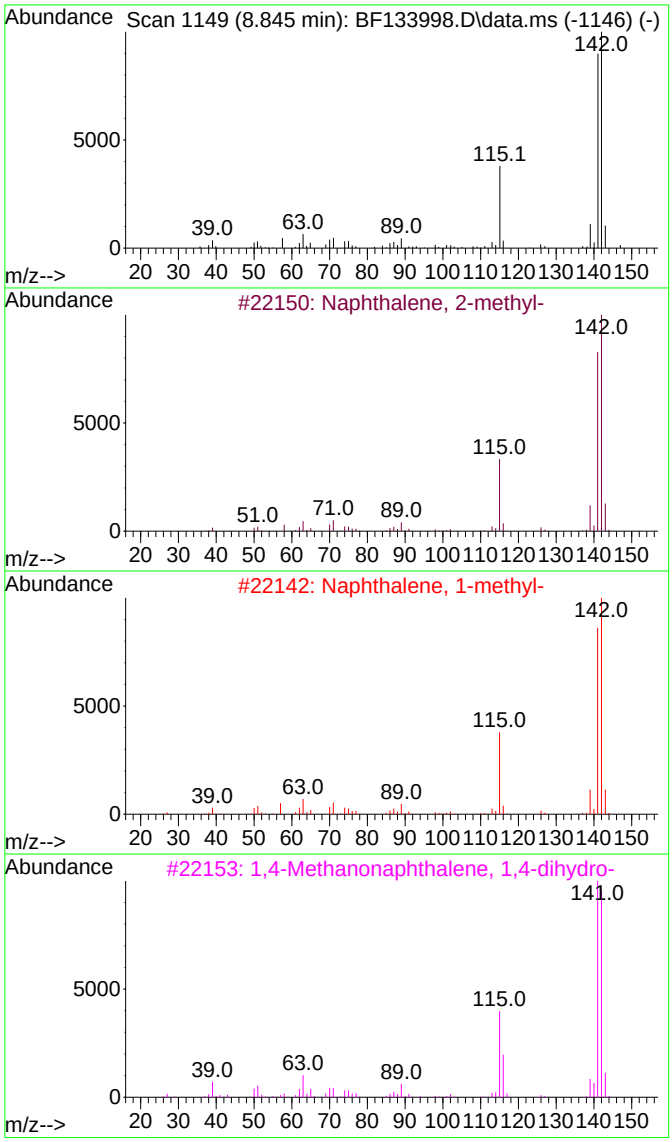
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

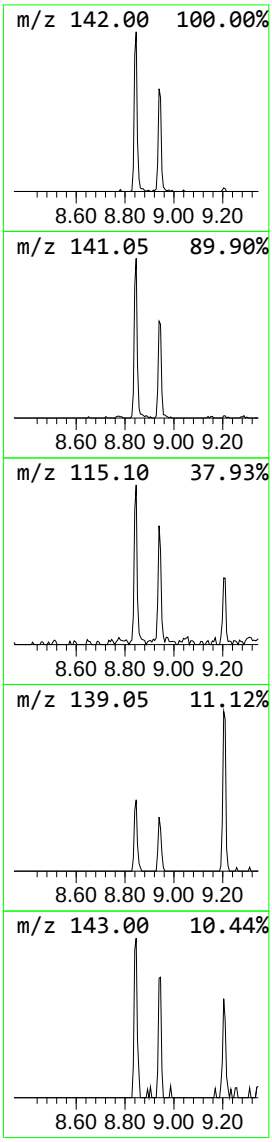
****

Peak Number 3 Naphthalene, 2-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.845	2.01 ng	75616	Naphthalene-d8	8.128

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
4	Benzocycloheptatriene	142	C11H10	000264-09-5	91
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062723\
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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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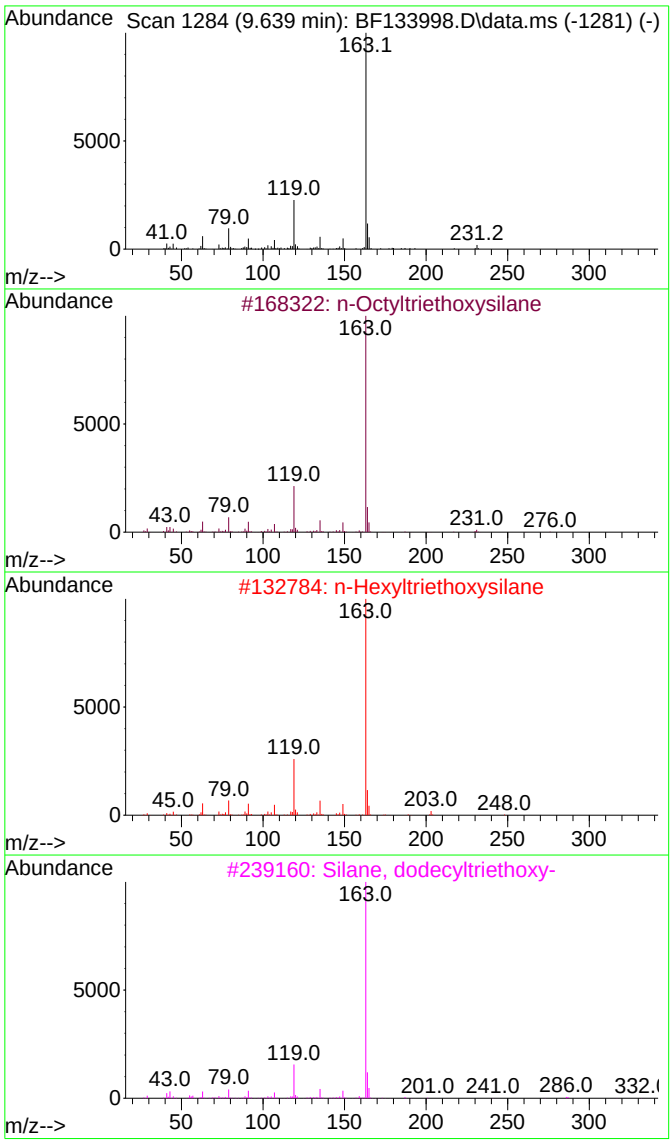
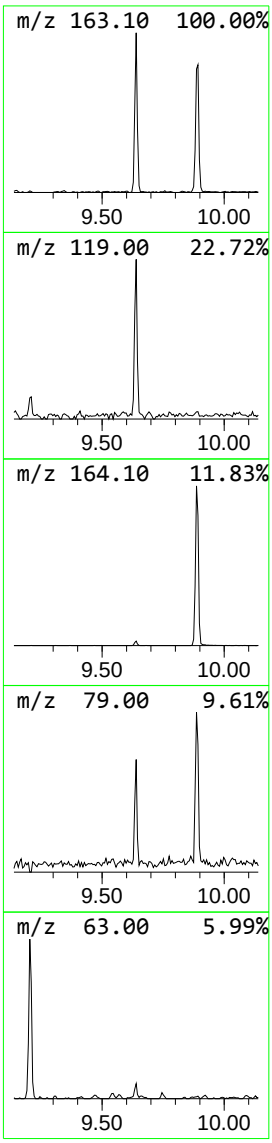
Peak Number 4 n-Octyltriethoxysilane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.639	2.02 ng	80284	Acenaphthene-d10	9.886

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Octyltriethoxysilane	276	C14H32O3Si	002943-75-1	91
2	n-Hexyltriethoxysilane	248	C12H28O3Si	018166-37-5	91
3	Silane, dodecyltriethoxy-	332	C18H40O3Si	018536-91-9	86
4	Octadecyltriethoxysilane	416	C24H52O3Si	007399-00-0	83
5	1H,1H,2H,2H-Perfluorooctyltrieth...	510	C14H19F13O3Si	051851-37-7	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062723\
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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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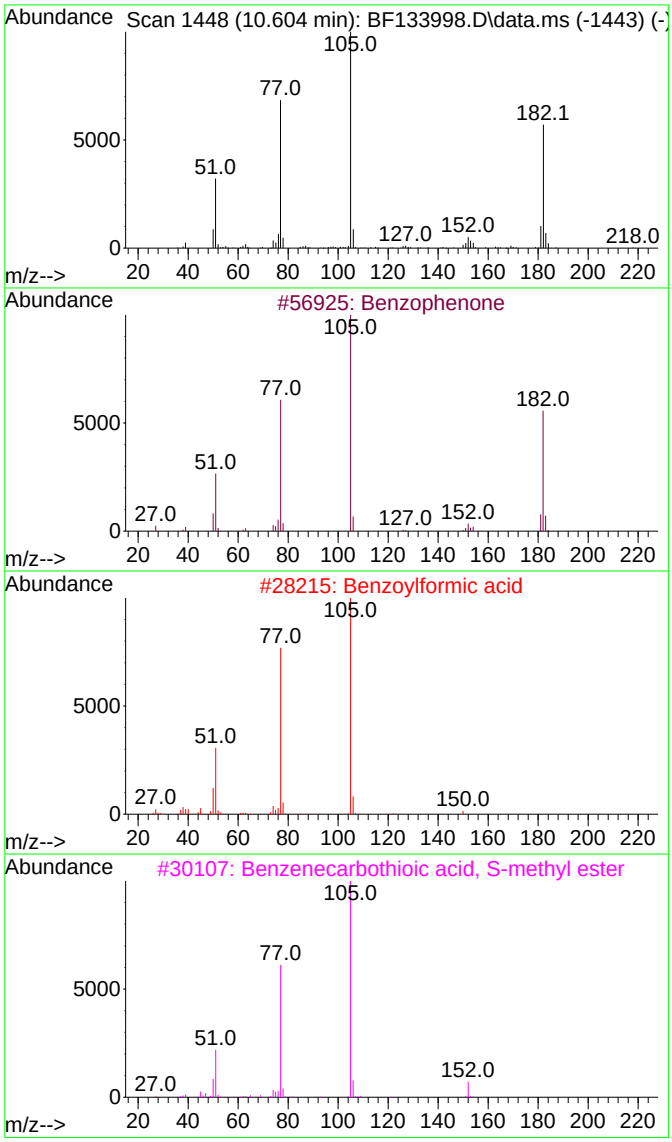
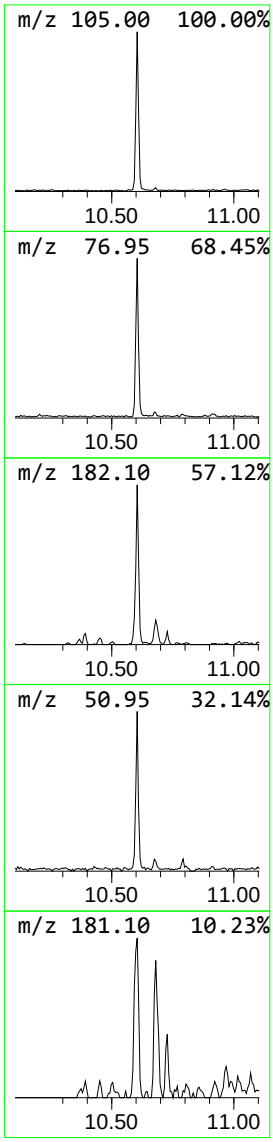
Peak Number 5 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.604	4.22 ng	167519	Acenaphthene-d10	9.886

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Benzoylformic acid	150	C8H6O3	000611-73-4	49
3	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	47
4	Ethanedione, diphenyl-	210	C14H10O2	000134-81-6	43
5	N-cyanobenzamide	146	C8H6N2O	015150-25-1	43





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ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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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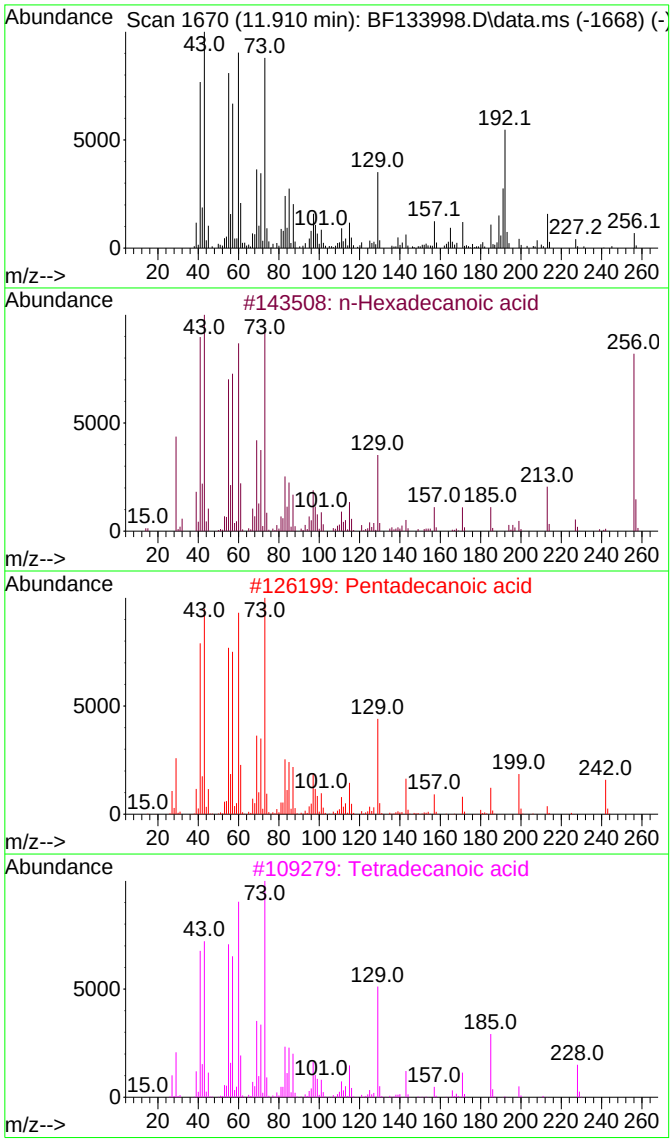
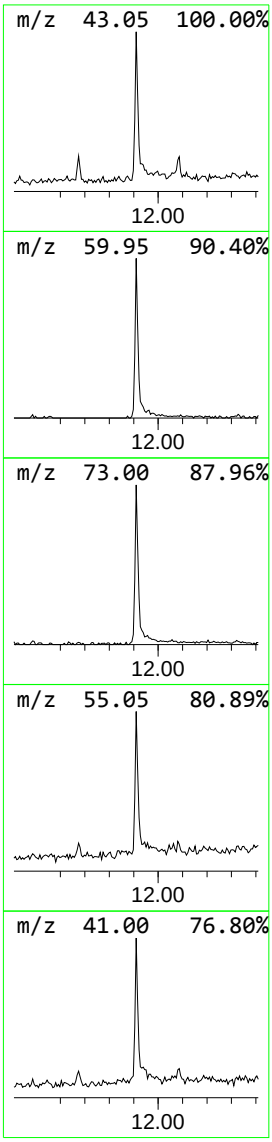
Peak Number 6 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.910	6.63 ng	227869	Phenanthrene-d10	11.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	70
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4	n-Decanoic acid	172	C10H20O2	000334-48-5	55
5	Tridecanoic acid	214	C13H26O2	000638-53-9	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062723\
Data File : BF133998.D
Acq On : 27 Jun 2023 19:03
Operator : CG\JU
Sample : 03402-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1-0623

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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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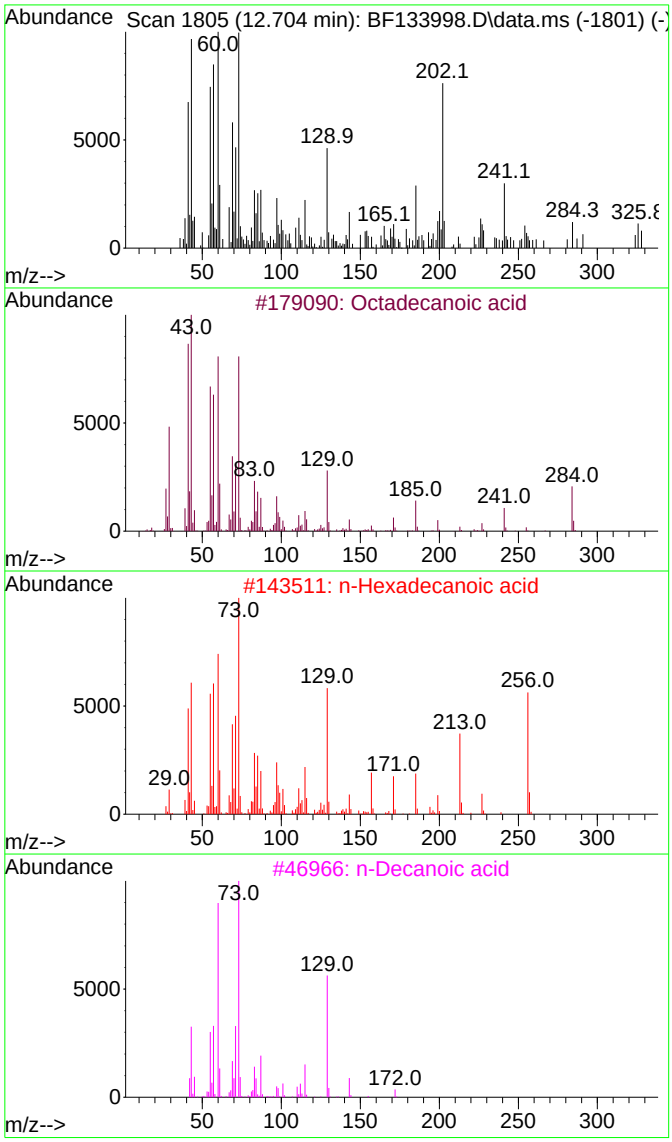
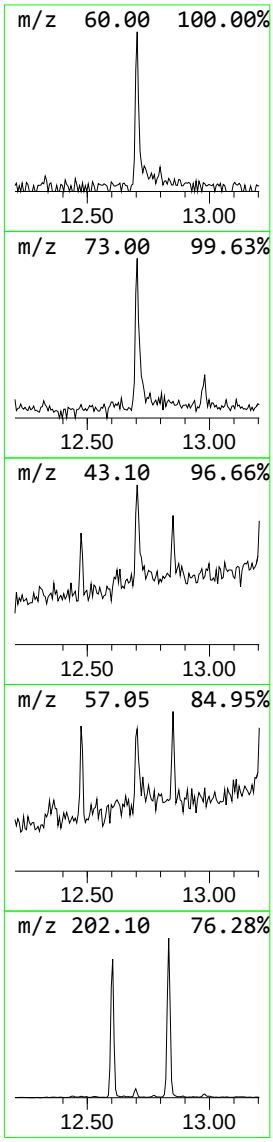
Peak Number 7 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.704	2.31 ng	79562	Phenanthrene-d10	11.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	97
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	70
3	n-Decanoic acid	172	C10H20O2	000334-48-5	47
4	Dodecanoic acid	200	C12H24O2	000143-07-7	46
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062723\
Data File : BF133998.D
Acq On : 27 Jun 2023 19:03
Operator : CG\JU
Sample : 03402-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1-0623

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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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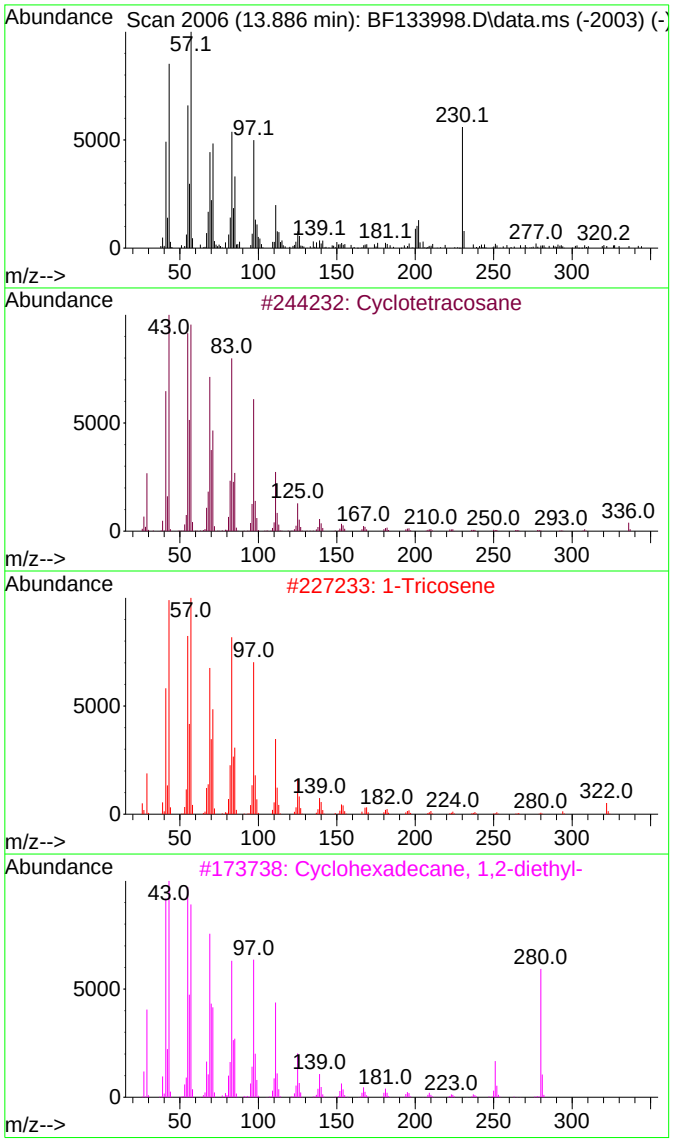
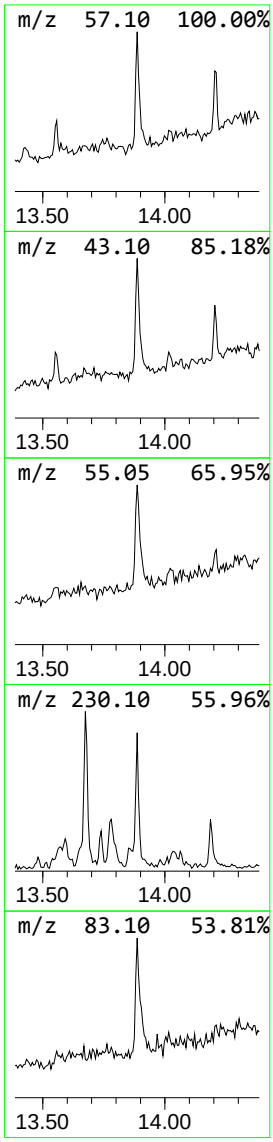
Peak Number 8 Cyclotetracosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	6.05 ng	194962	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	95
2	1-Tricosene	322	C23H46	018835-32-0	91
3	Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	83
4	1-Octadecene	252	C18H36	000112-88-9	70
5	9-Tricosene, (Z)-	322	C23H46	027519-02-4	64





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Operator : CG\JU
Sample : 03402-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1-0623

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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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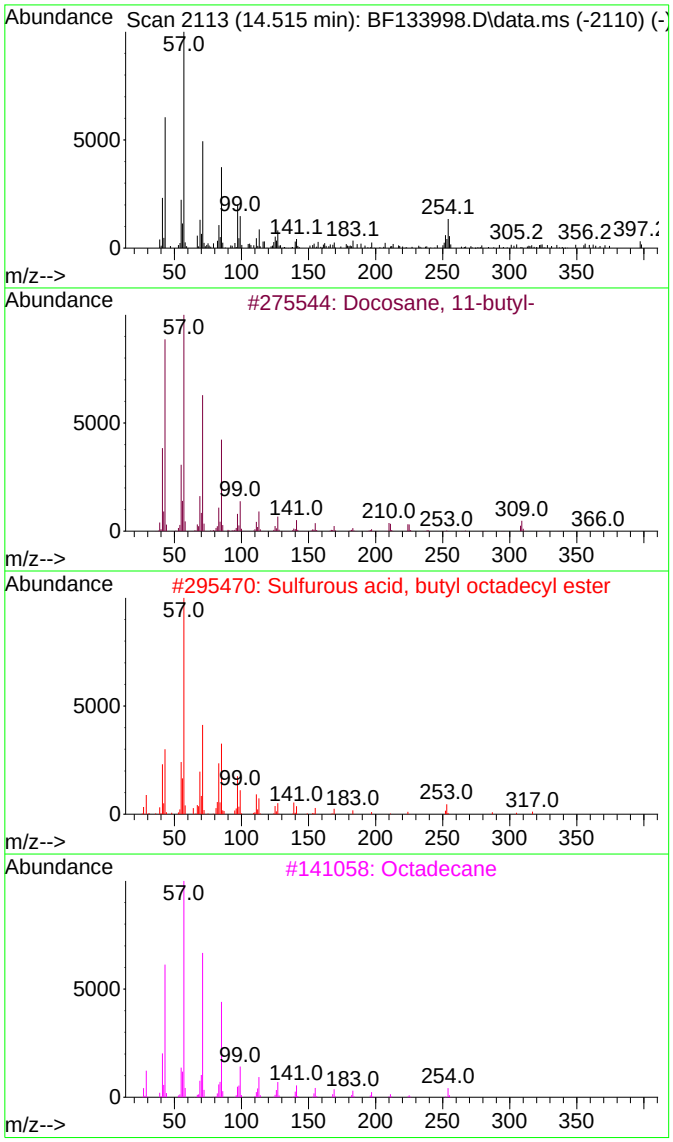
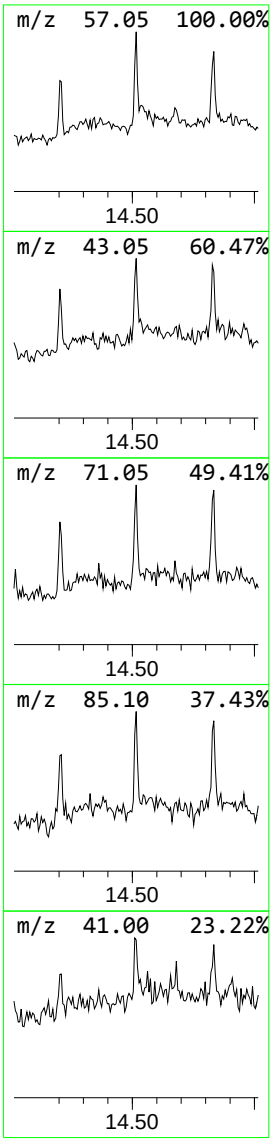
Peak Number 9 Docosane, 11-butyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.515	3.37 ng	108368	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane, 11-butyl-	366	C26H54	013475-76-8	86
2	Sulfurous acid, butyl octadecyl ...	390	C22H46O3S	1000309-18-5	80
3	Octadecane	254	C18H38	000593-45-3	76
4	Tricosane	324	C23H48	000638-67-5	70
5	Docosane, 9-butyl-	366	C26H54	055282-14-9	64





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Data File : BF133998.D
Acq On : 27 Jun 2023 19:03
Operator : CG\JU
Sample : 03402-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1-0623

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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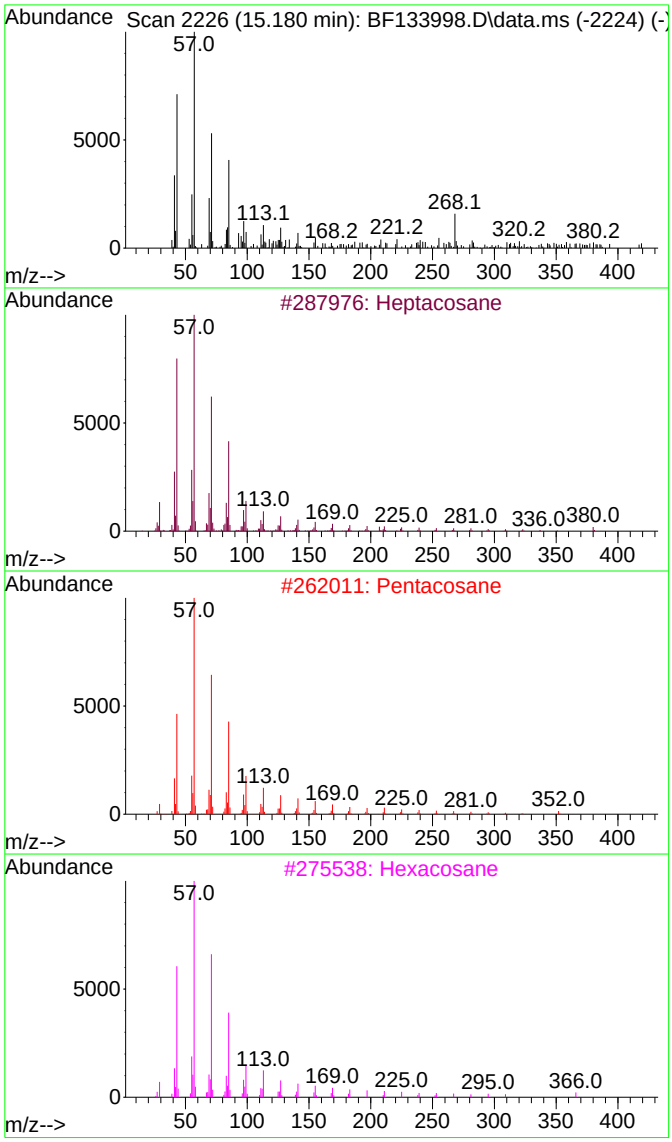
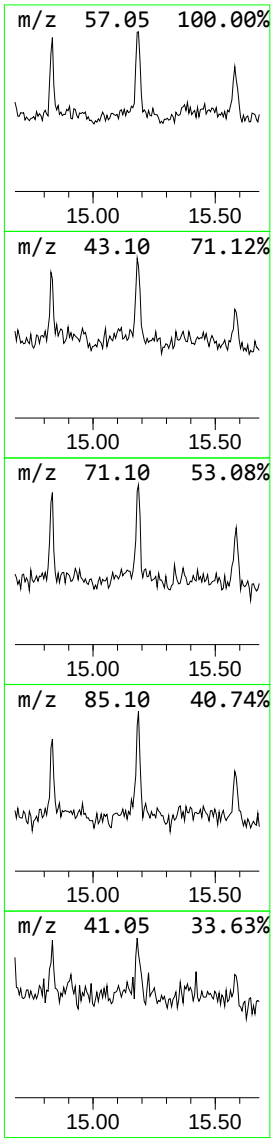
Peak Number 10 Heptacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.180	4.84 ng	84280	Perylene-d12	15.545

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	86
2	Pentacosane	352	C25H52	000629-99-2	86
3	Hexacosane	366	C26H54	000630-01-3	70
4	Nonadecane	268	C19H40	000629-92-5	64
5	Hexadecane, 7,9-dimethyl-	254	C18H38	021164-95-4	62





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Operator : CG\JU
Sample : 03402-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1-0623

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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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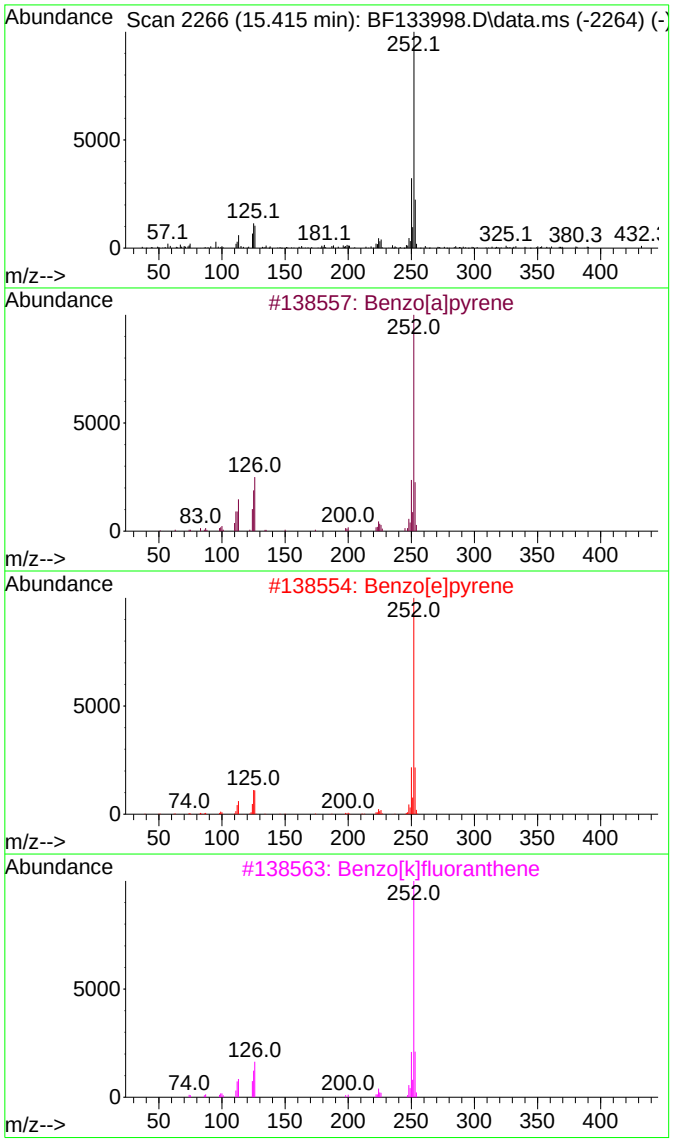
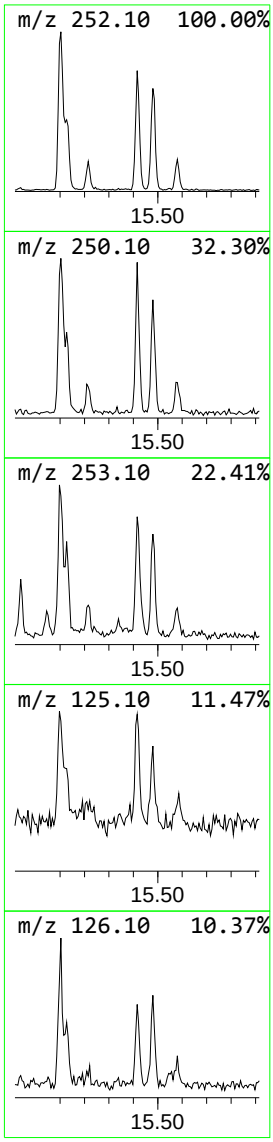
Peak Number 11 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.415	6.26 ng	109136	Perylene-d12	15.545

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[a]pyrene	252	C20H12	000050-32-8	95
2	Benzo[e]pyrene	252	C20H12	000192-97-2	95
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	94
4	Perylene	252	C20H12	000198-55-0	90
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	89





Tentatively Identified Compound (LSC) summary

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Data File : BF133998.D
Acq On : 27 Jun 2023 19:03
Operator : CG\JU
Sample : 03402-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP1-0623

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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...	2.169	41.8	ng	1418280	1	6.851	679459	20.0
2-Pentanone, 4-...	5.093	3.2	ng	108532	1	6.851	679459	20.0
Naphthalene, 2-...	8.845	2.0	ng	75616	2	8.128	750816	20.0
n-Octyltriethox...	9.639	2.0	ng	80284	3	9.886	794615	20.0
Benzophenone	10.604	4.2	ng	167519	3	9.886	794615	20.0
n-Hexadecanoic ...	11.910	6.6	ng	227869	4	11.380	687584	20.0
Octadecanoic acid	12.704	2.3	ng	79562	4	11.380	687584	20.0
Cyclotetracosane	13.886	6.0	ng	194962	5	14.039	643995	20.0
Docosane, 11-bu...	14.515	3.4	ng	108368	5	14.039	643995	20.0
Heptacosane	15.180	4.8	ng	84280	6	15.545	348449	20.0
Benzo[e]pyrene	15.415	6.3	ng	109136	6	15.545	348449	20.0