LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082521\
Data File : BF125208.D
Acq On : 25 Aug 2021 14:15
Operator : JU/CG
Sample : M3523-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11998

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-BF081821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125208.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.210	15	21	27	rVB	921235	1153044	33.96%	3.120%
2	5.139	511	519	526	rBV	66237	87170	2.57%	0.236%
3	5.534	581	586	589	rBV	2923647	2945176	86.74%	7.970%
4	6.534	751	756	759	rBV	3050008	2961008	87.20%	8.013%
5	6.916	817	821	824	rBV	993124	869197	25.60%	2.352%
6	7.475	911	916	919	rBV	2254470	1951328	57.47%	5.280%
7	8.098	1018	1022	1035	rBV	63121	154445	4.55%	0.418%
8	8.198	1035	1039	1042	rBV	1306827	1139498	33.56%	3.083%
9	8.904	1156	1159	1163	rBV	137707	125593	3.70%	0.340%
10	9.004	1173	1176	1183	rVB	99975	84968	2.50%	0.230%
11	9.269	1217	1221	1224	rBV	4025154	3395529	100.00%	9.188%
12	9.369	1235	1238	1242	rVB	128824	99211	2.92%	0.268%
13	9.539	1260	1267	1271	rBV2	51930	69999	2.06%	0.189%
14	9.604	1276	1278	1281	rVV	68579	61597	1.81%	0.167%
15	9.951	1330	1337	1340	rBV	1536307	1285048	37.85%	3.477%
16	9.980	1340	1342	1346	rVB	767424	647726	19.08%	1.753%
17	10.151	1367	1371	1375	rBV	619504	552943	16.28%	1.496%
18	10.351	1401	1405	1407	rBV2	42192	38301	1.13%	0.104%
19	10.498	1426	1430	1435	rBV	833015	665257	19.59%	1.800%
20	10.586	1443	1445	1447	rVB	78664	60445	1.78%	0.164%
21	10.627	1450	1452	1454	rVV2	50851	50272	1.48%	0.136%
22	10.651	1454	1456	1460	rVB	128451	109394	3.22%	0.296%
23	10.739	1467	1471	1474	rBV	2647843	2293041	67.53%	6.205%
24	10.863	1485	1492	1495	rVB2	59229	62006	1.83%	0.168%
25	11.045	1516	1523	1526	rBV3	85109	105381	3.10%	0.285%
26	11.239	1553	1556	1560	rVV	103198	86134	2.54%	0.233%
27	11.280	1560	1563	1568	rVV2	37874	51798	1.53%	0.140%
28	11.333	1568	1572	1577	rVB	264589	216000	6.36%	0.584%
29	11.439	1586	1590	1592	rBV	1415527	1282478	37.77%	3.470%
30	11.463	1592	1594	1598	rVV	2980431	2566032	75.57%	6.944%
31	11.510	1600	1602	1605	rVB	181869	153955	4.53%	0.417%
32	11.663	1626	1628	1631	rBV	87409	77653	2.29%	0.210%
33	11.733	1637	1640	1644	rBV	52383	40727	1.20%	0.110%
34	11.939	1672	1675	1676	rBV	172879	152613	4.49%	0.413%
35	11.957	1676	1678	1683	rVB2	489762	534258	15.73%	1.446%
36	12.051	1690	1694	1697	rBV	362616	358449	10.56%	0.970%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082521\
Data File : BF125208.D
Acq On : 25 Aug 2021 14:15
Operator : JU/CG
Sample : M3523-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11998

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-BF081821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.074	1697	1698	1703	rVB	84752	46459	1.37%	0.126%
38	12.233	1722	1725	1727	rBV	153664	123350	3.63%	0.334%
39	12.257	1727	1729	1733	rVB	79434	62040	1.83%	0.168%
40	12.527	1771	1775	1780	rVB4	32335	42613	1.25%	0.115%
41	12.651	1792	1796	1800	rBV	1771989	1602291	47.19%	4.336%
42	12.739	1809	1811	1816	rBV	252997	268977	7.92%	0.728%
43	12.804	1820	1822	1826	rVV	54807	46716	1.38%	0.126%
44	12.880	1829	1835	1839	rVV	1216152	1308378	38.53%	3.540%
45	12.927	1839	1843	1848	rVB	46304	56828	1.67%	0.154%
46	13.021	1855	1859	1863	rVB	3335662	2951889	86.93%	7.988%
47	13.098	1867	1872	1876	rBV3	39237	65271	1.92%	0.177%
48	13.186	1879	1887	1888	rBV3	30706	42969	1.27%	0.116%
49	13.210	1888	1891	1894	rVB	122967	111296	3.28%	0.301%
50	13.274	1899	1902	1905	rVB	128415	94589	2.79%	0.256%
51	13.310	1905	1908	1911	rBV2	58031	61053	1.80%	0.165%
52	13.827	1989	1996	1998	rBV2	39800	45637	1.34%	0.123%
53	13.857	1998	2001	2002	rVV	61889	57291	1.69%	0.155%
54	13.874	2002	2004	2008	rVV3	74891	88288	2.60%	0.239%
55	13.915	2008	2011	2014	rVV2	92399	123315	3.63%	0.334%
56	13.945	2014	2016	2018	rVV	117322	100749	2.97%	0.273%
57	13.998	2018	2025	2032	rVV7	64672	210920	6.21%	0.571%
58	14.080	2033	2039	2041	rVV2	959577	1147301	33.79%	3.105%
59	14.104	2041	2043	2049	rVB	194679	175741	5.18%	0.476%
60	14.233	2061	2065	2072	rVB3	42114	56740	1.67%	0.154%
61	14.539	2114	2117	2122	rBV3	50293	57463	1.69%	0.155%
62	14.856	2165	2171	2174	rVB4	49924	65702	1.93%	0.178%
63	14.939	2181	2185	2189	rBV	37957	43040	1.27%	0.116%
64	15.133	2213	2218	2221	rBV	86196	131469	3.87%	0.356%
65	15.209	2227	2231	2235	rBV2	44900	50306	1.48%	0.136%
66	15.445	2267	2271	2275	rBV	44050	47323	1.39%	0.128%
67	15.504	2278	2281	2284	rBV	44122	53668	1.58%	0.145%
68	15.574	2288	2293	2302	rVB	715305	940523	27.70%	2.545%
69	16.051	2370	2374	2379	rVB2	47826	75984	2.24%	0.206%
70	16.574	2459	2463	2470	rBV2	26291	49597	1.46%	0.134%
71	17.192	2563	2568	2575	rVB3	31709	61262	1.80%	0.166%

Sum of corrected areas: 36954712

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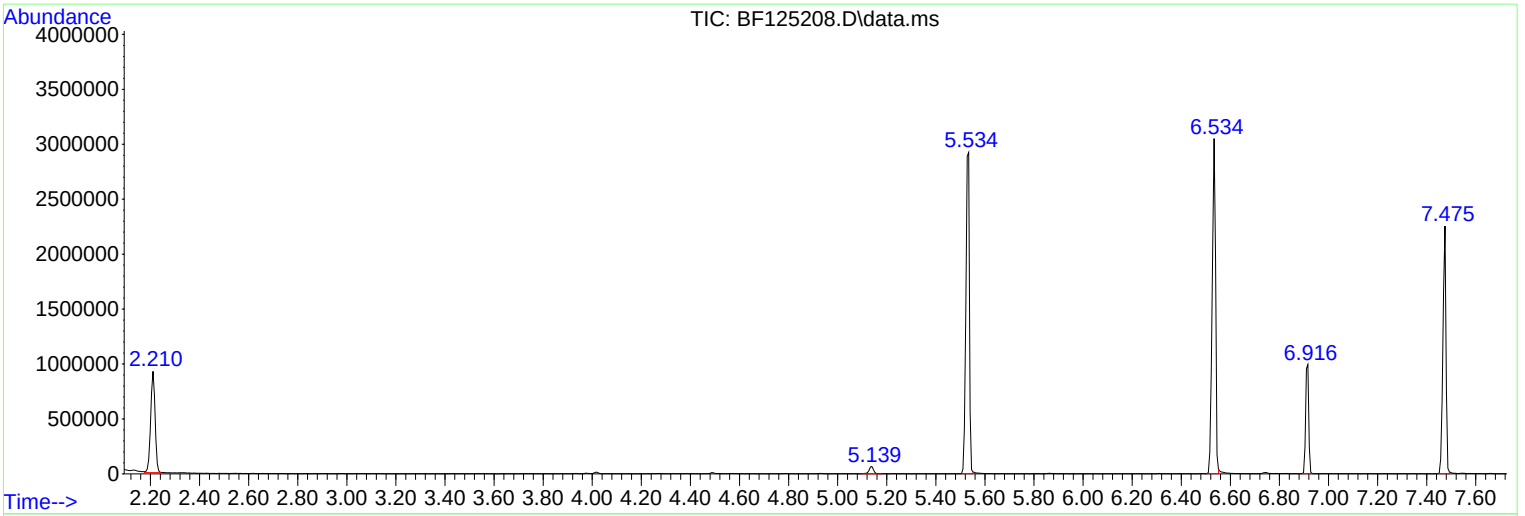
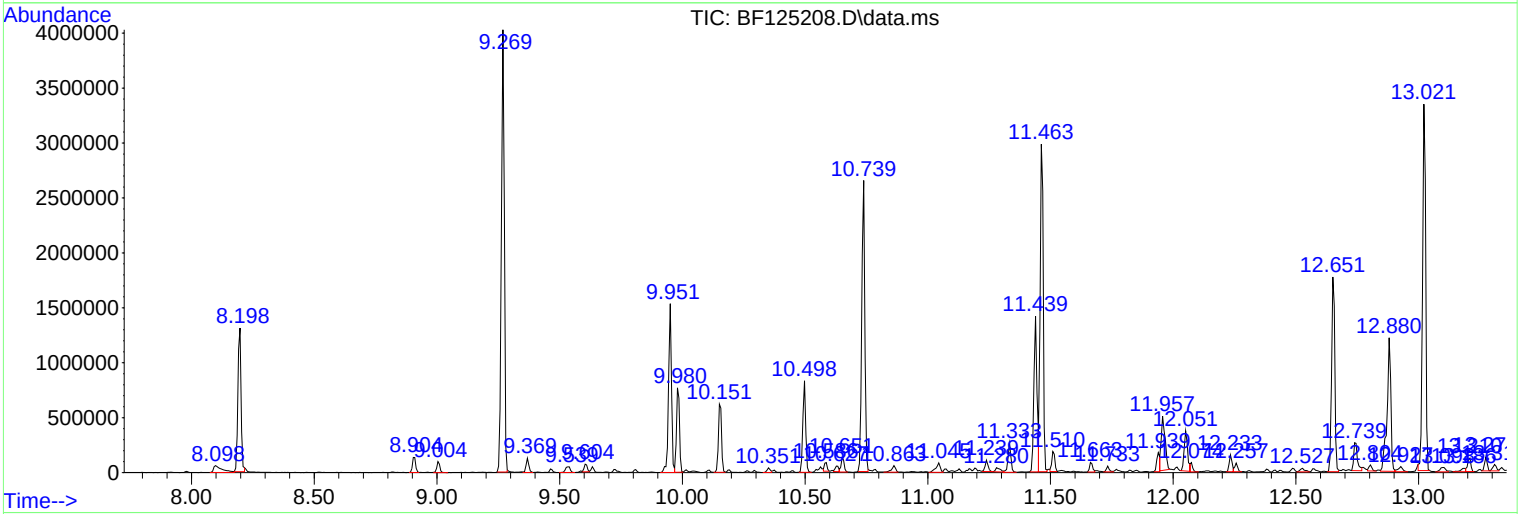
Sample : M3523-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

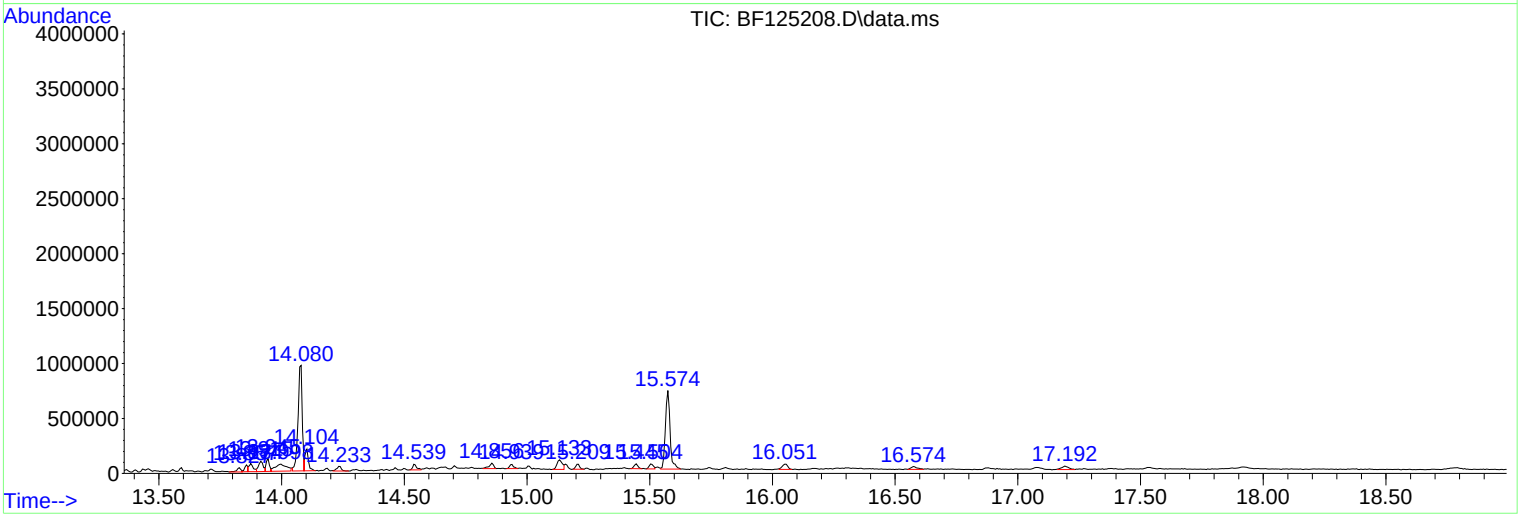
Instrument :
BNA_F
ClientSampleId :
72-11998

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.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\BF082521\
Data File : BF125208.D
Acq On : 25 Aug 2021 14:15
Operator : JU/CG
Sample : M3523-01
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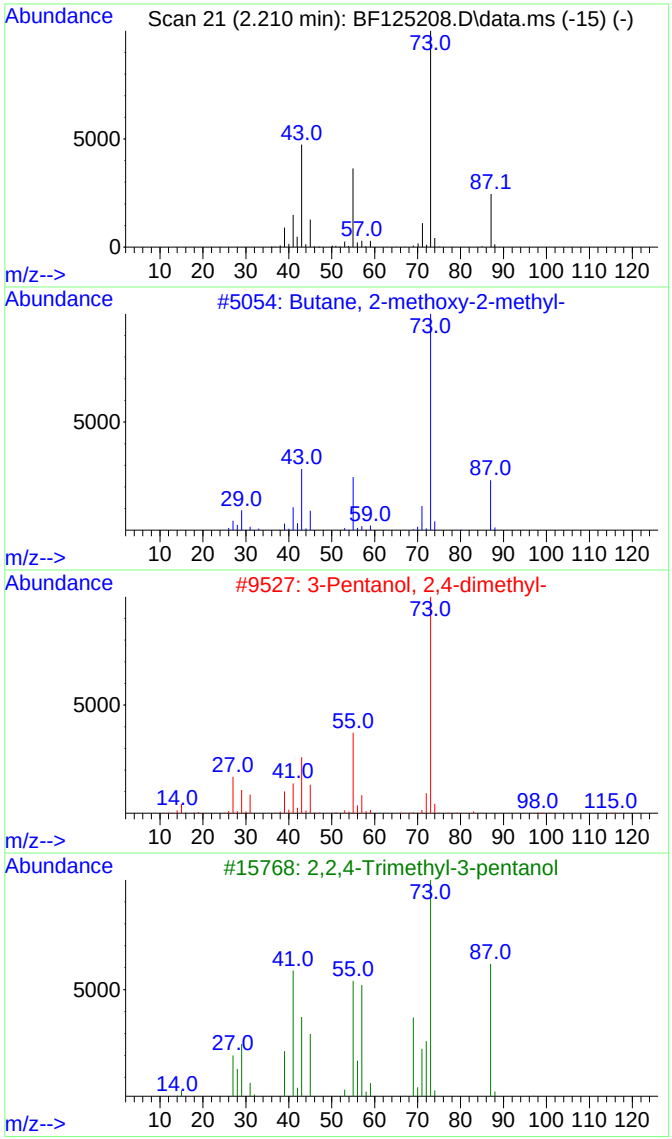
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

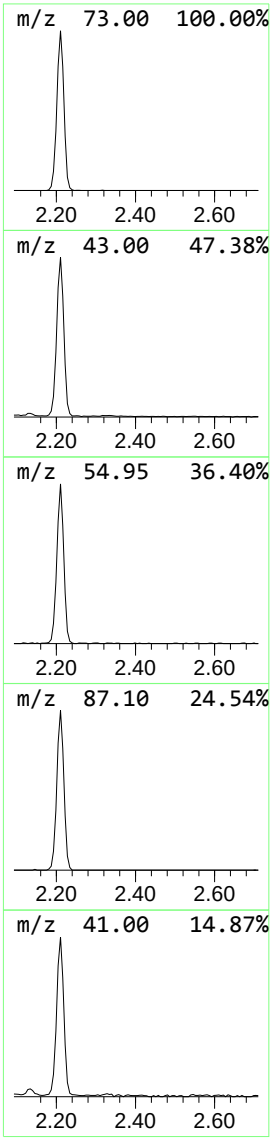
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.210	26.53 ng	1153040	1,4-Dichlorobenzene-d4	6.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082521\
Data File : BF125208.D
Acq On : 25 Aug 2021 14:15
Operator : JU/CG
Sample : M3523-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11998

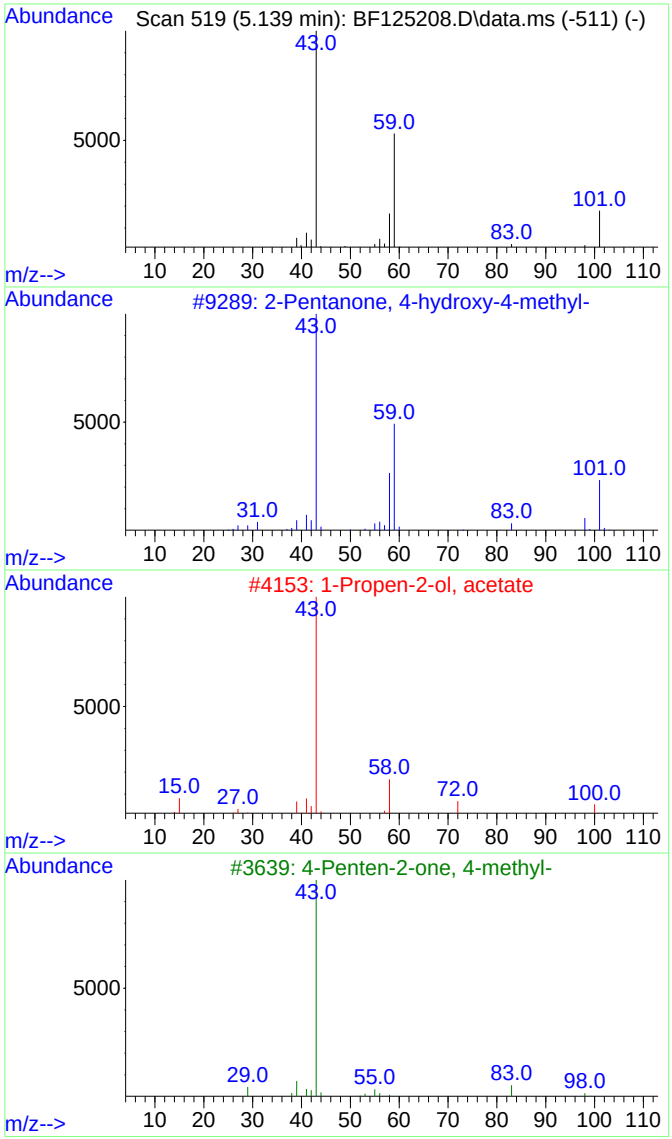
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

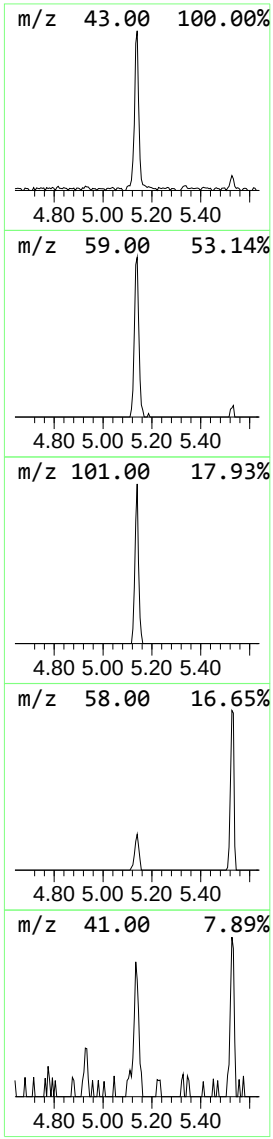
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.139	2.01 ng	87170	1,4-Dichlorobenzene-d4	6.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
5	Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	5





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082521\
Data File : BF125208.D
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Sample : M3523-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11998

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

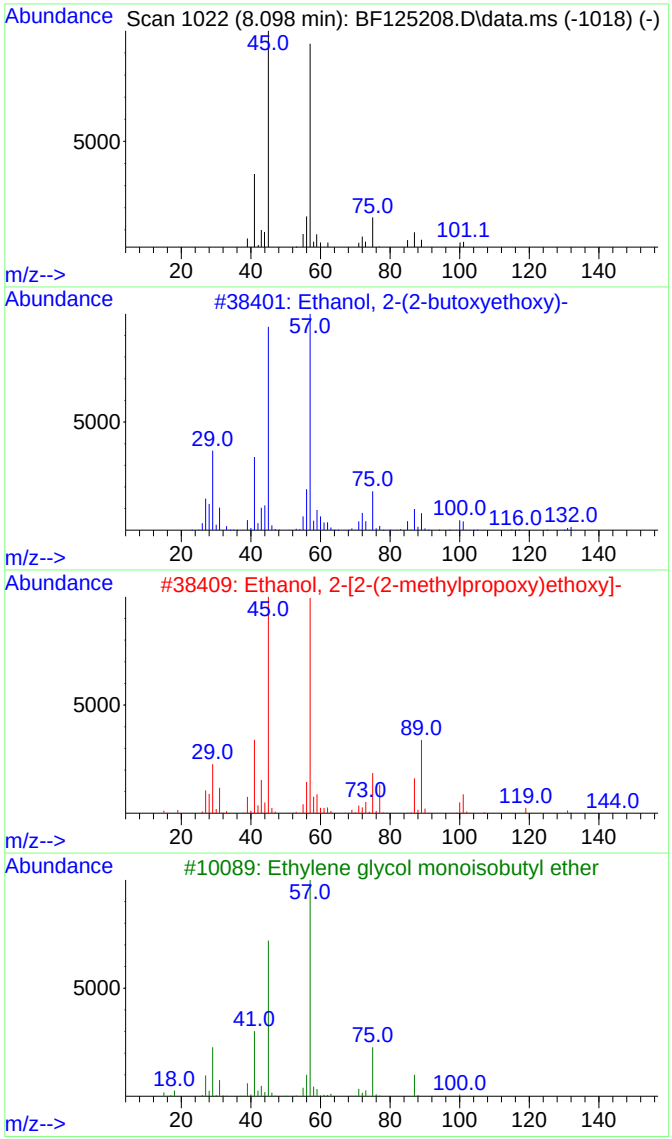
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

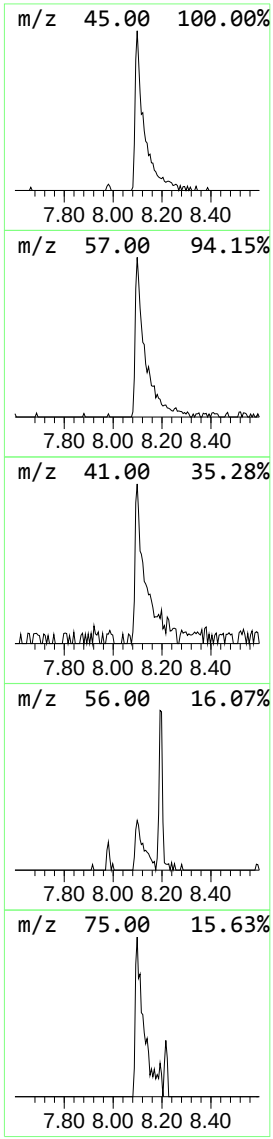
****

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.098	2.71 ng	154445	Naphthalene-d8	8.198

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	83
2	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	64
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	50
4	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	45
5	1-Methoxy-3-methyl-3-butene	100	C6H12O	034752-58-4	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082521\
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Misc :
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Instrument :
BNA_F
ClientSampleId :
72-11998

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

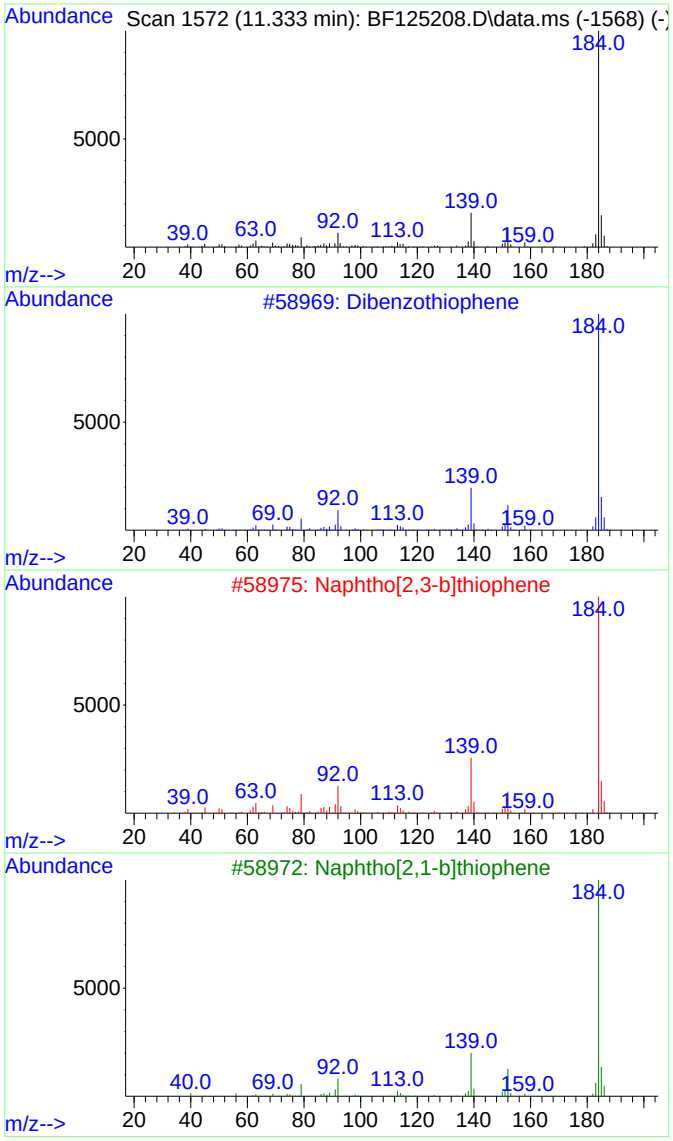
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

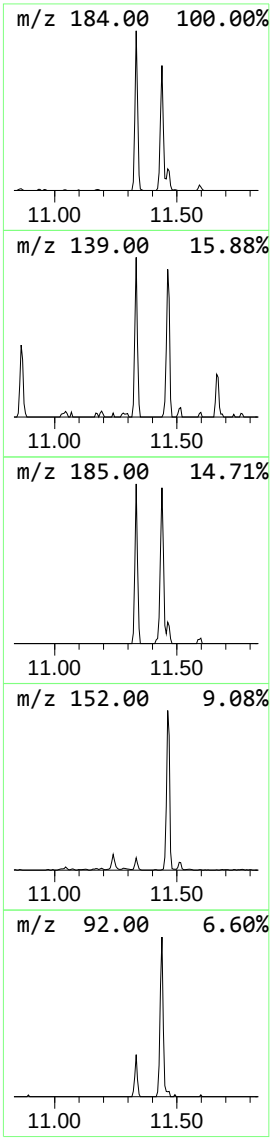
****

Peak Number 4 Dibenzothiophene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.333	3.37 ng	216000	Phenanthrene-d10	11.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibenzothiophene	184	C12H8S	000132-65-0	97
2	Naphtho[2,3-b]thiophene	184	C12H8S	000268-77-9	95
3	Naphtho[2,1-b]thiophene	184	C12H8S	000233-02-3	95
4	Naphtho[1,2-b]thiophene	184	C12H8S	000234-41-3	94
5	Azuleno(2,1-b)thiophene	184	C12H8S	000248-13-5	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082521\
Data File : BF125208.D
Acq On : 25 Aug 2021 14:15
Operator : JU/CG
Sample : M3523-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11998

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

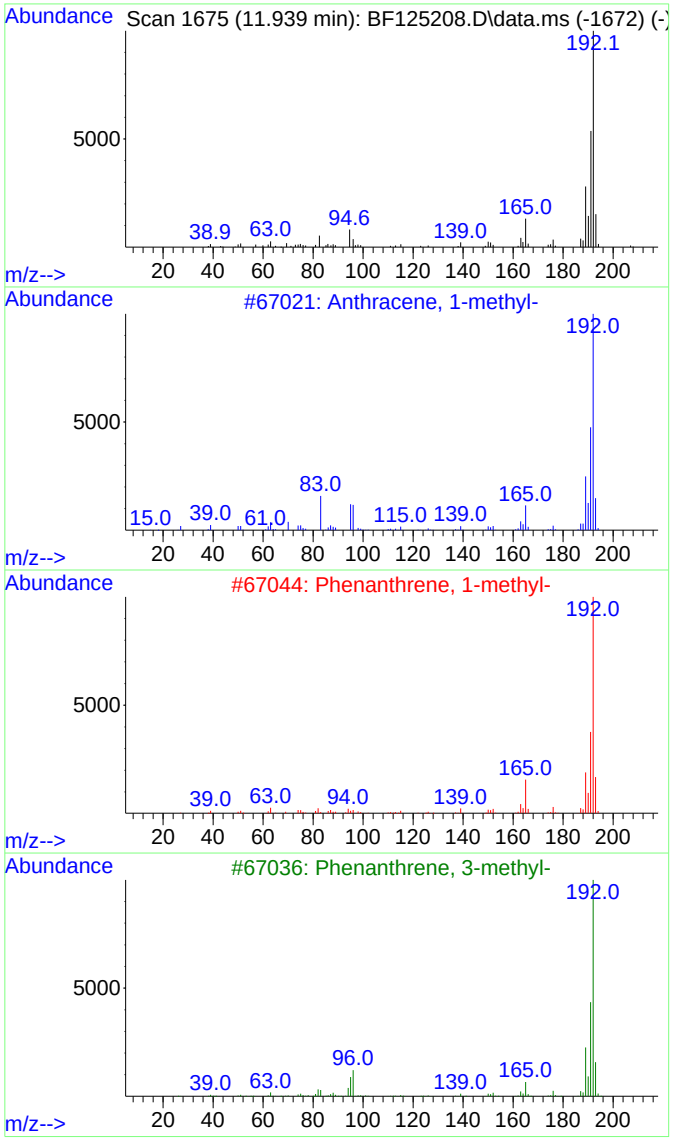
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

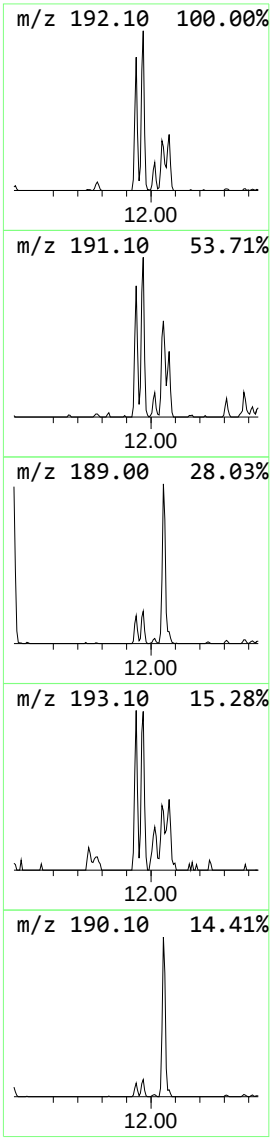
****

Peak Number 5 Anthracene, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.939	2.38 ng	152613	Phenanthrene-d10	11.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 1-methyl-	192	C15H12	000610-48-0	94
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	94
3	Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	94
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	94
5	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082521\
Data File : BF125208.D
Acq On : 25 Aug 2021 14:15
Operator : JU/CG
Sample : M3523-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11998

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

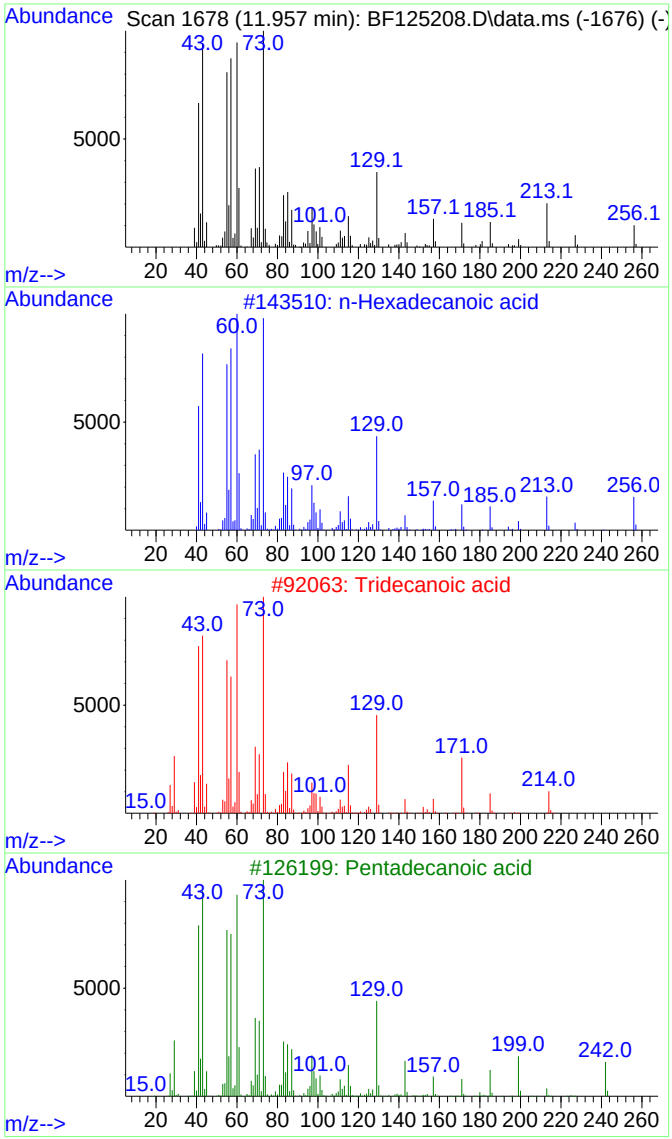
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

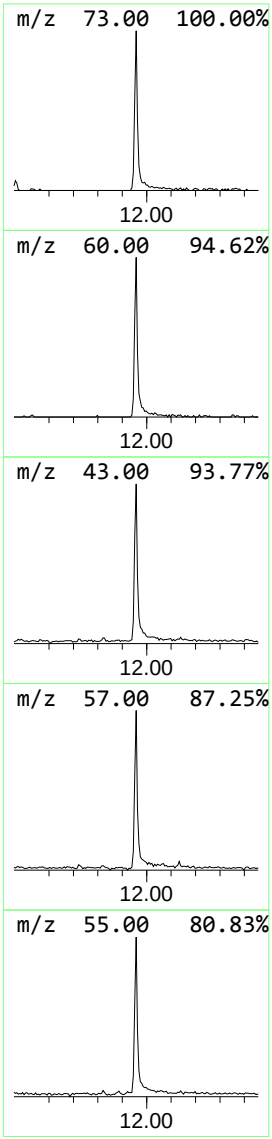
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.957	8.33 ng	534258	Phenanthrene-d10	11.439

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	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	70
5	Undecanoic acid	186	C11H22O2	000112-37-8	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082521\
Data File : BF125208.D
Acq On : 25 Aug 2021 14:15
Operator : JU/CG
Sample : M3523-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11998

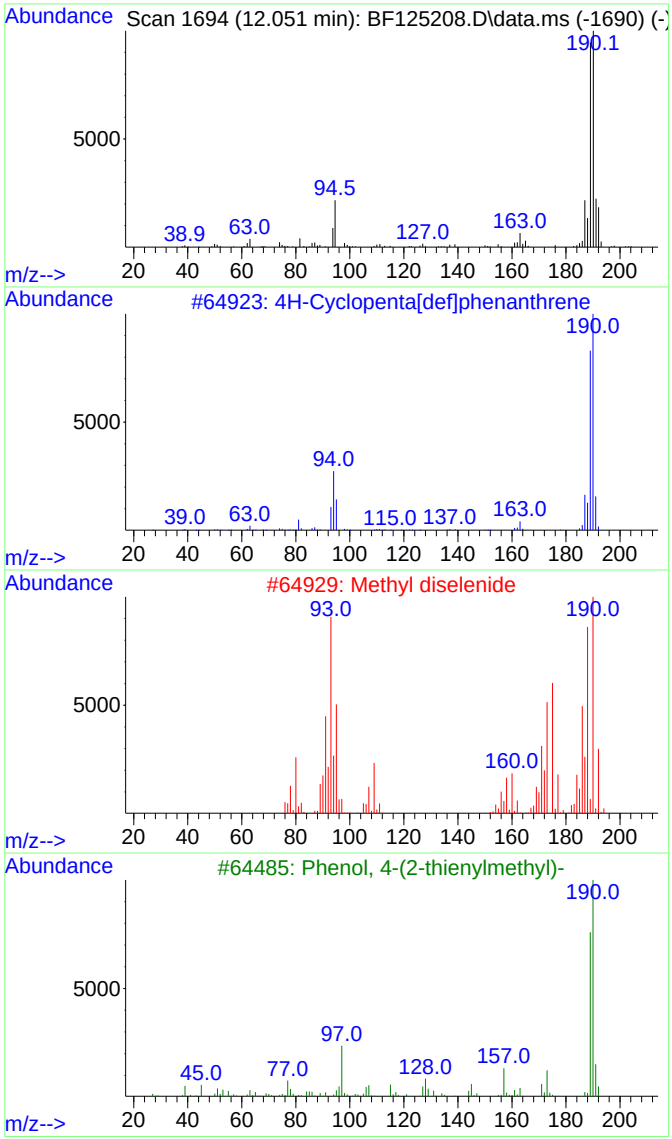
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

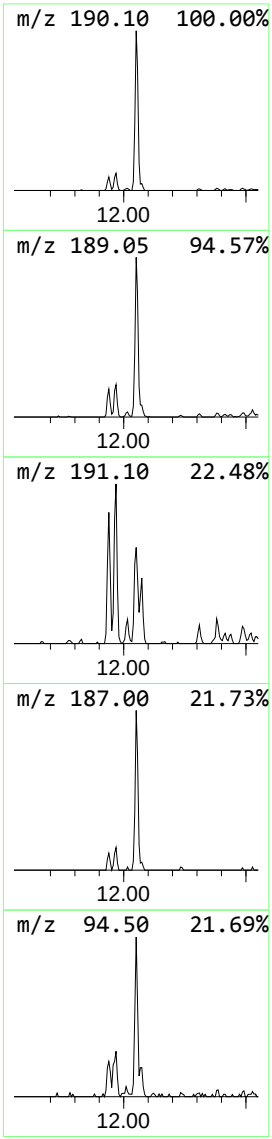
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 4H-Cyclopenta[def]phenanthrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.051	5.59 ng	358449	Phenanthrene-d10	11.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	97
2	Methyl diselenide	190	C2H6Se2	007101-31-7	46
3	Phenol, 4-(2-thienylmethyl)-	190	C11H10OS	091680-55-6	45
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	45
5	Cyclohexanone, 2-(2-furanylmethy...	190	C12H14O2	056053-07-7	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082521\
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Acq On : 25 Aug 2021 14:15
Operator : JU/CG
Sample : M3523-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11998

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.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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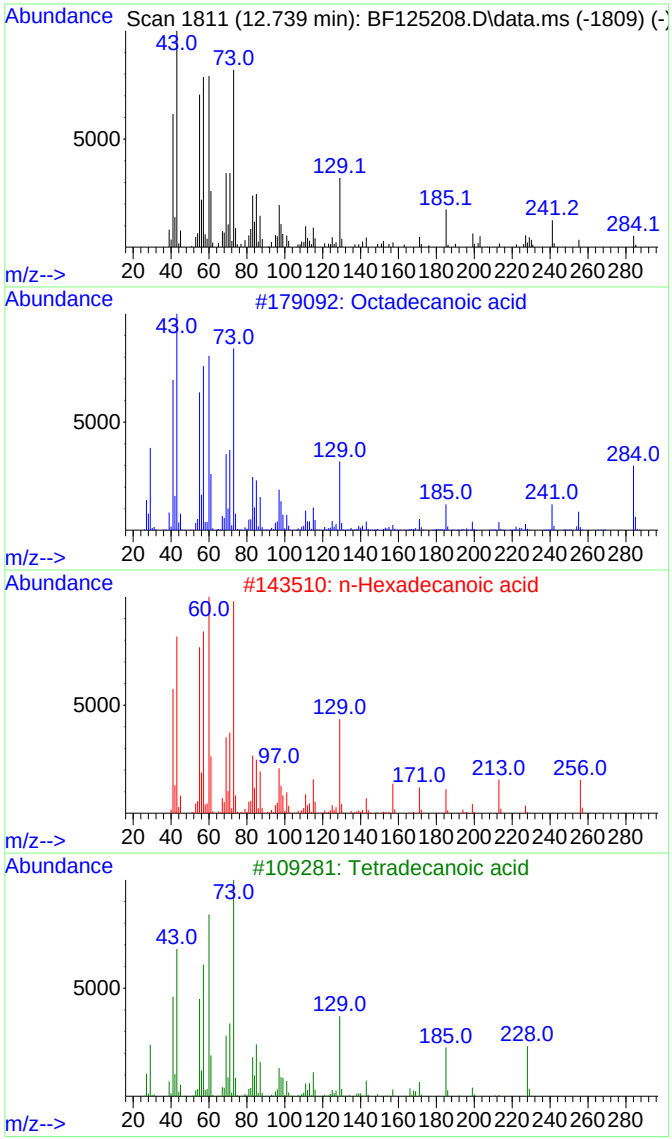
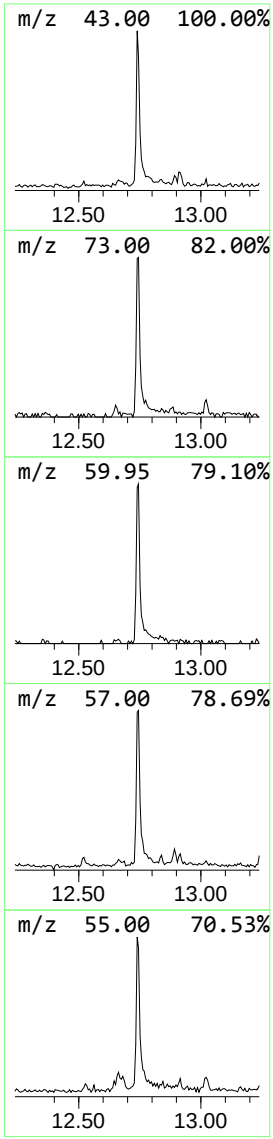
Peak Number 8 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.739	4.19 ng	268977	Phenanthrene-d10	11.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	n-Decanoic acid	172	C10H20O2	000334-48-5	58
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	49





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Data File : BF125208.D
Acq On : 25 Aug 2021 14:15
Operator : JU/CG
Sample : M3523-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11998

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.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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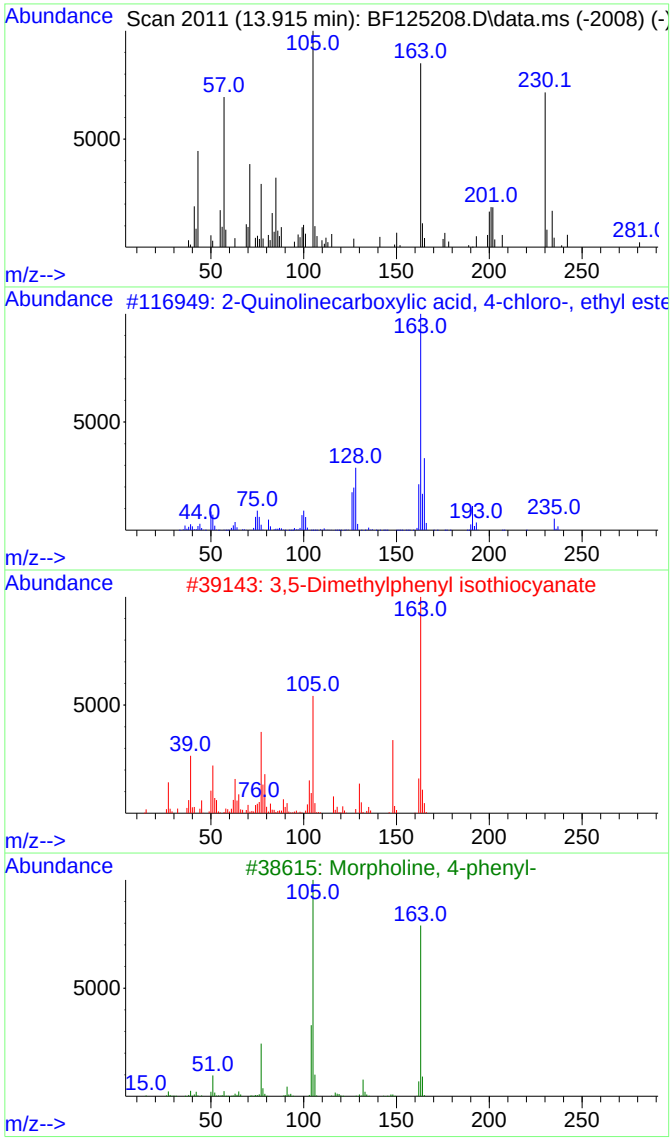
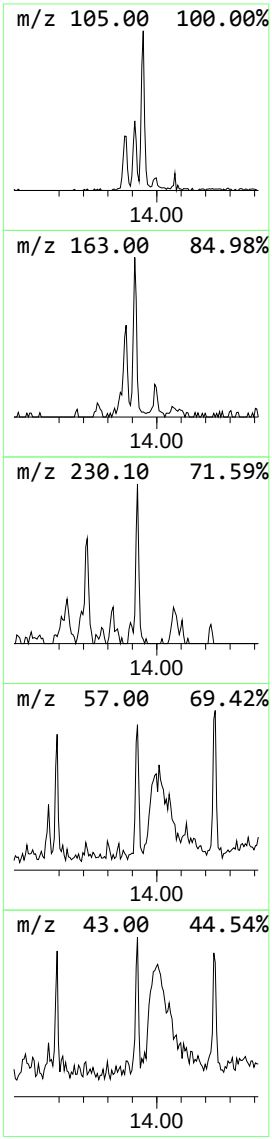
Peak Number 9 unknown13.915 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.915	2.15 ng	123315	Chrysene-d12	14.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Quinolinecarboxylic acid, 4-ch...	235	C12H10ClNO2	1000351-34-0	30
2	3,5-Dimethylphenyl isothiocyanate	163	C9H9NS	040046-30-8	25
3	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	22
4	2,3-Dihydro-4-methoxyindole-2-one	163	C9H9NO2	007699-17-4	22
5	11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	18





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082521\
Data File : BF125208.D
Acq On : 25 Aug 2021 14:15
Operator : JU/CG
Sample : M3523-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11998

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.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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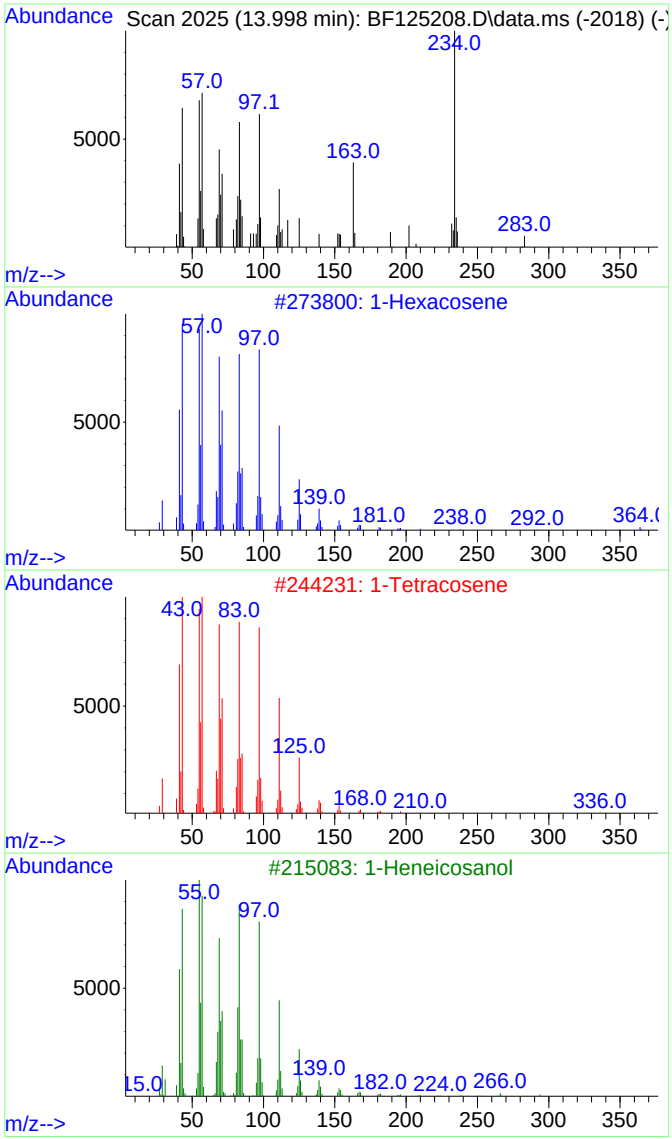
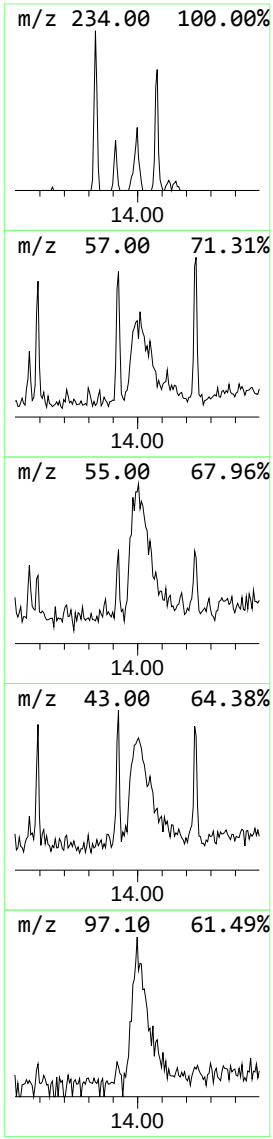
Peak Number 10 unknown13.998 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.998	3.68 ng	210920	Chrysene-d12	14.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene	364	C26H52	018835-33-1	42
2	1-Tetracosene	336	C24H48	010192-32-2	42
3	1-Heneicosanol	312	C21H44O	015594-90-8	42
4	1-Docosene	308	C22H44	001599-67-3	38
5	1-Tricosene	322	C23H46	018835-32-0	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082521\
Data File : BF125208.D
Acq On : 25 Aug 2021 14:15
Operator : JU/CG
Sample : M3523-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11998

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.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...	2.210	26.5	ng	1153040	1	6.916	869197	20.0
2-Pentanone, 4-...	5.139	2.0	ng	87170	1	6.916	869197	20.0
Ethanol, 2-(2-b...	8.098	2.7	ng	154445	2	8.198	1139500	20.0
Dibenzothiophene	11.333	3.4	ng	216000	4	11.439	1282480	20.0
Anthracene, 1-m...	11.939	2.4	ng	152613	4	11.439	1282480	20.0
n-Hexadecanoic ...	11.957	8.3	ng	534258	4	11.439	1282480	20.0
4H-Cyclopenta[d...	12.051	5.6	ng	358449	4	11.439	1282480	20.0
Octadecanoic acid	12.739	4.2	ng	268977	4	11.439	1282480	20.0
unknown13.915	13.915	2.1	ng	123315	5	14.080	1147300	20.0
unknown13.998	13.998	3.7	ng	210920	5	14.080	1147300	20.0