LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050322\
Data File : BF128057.D
Acq On : 03 May 2022 20:38
Operator : CG\JU
Sample : N2659-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 22L097-B

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-BF042222.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128057.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.681	232	237	250	rVB	21503	33107	1.07%	0.186%
2	4.534	374	382	386	rBV	1386556	1527149	49.37%	8.583%
3	5.163	480	489	491	rBV	1964141	3093172	100.00%	17.384%
4	5.534	549	552	558	rVB	76597	70189	2.27%	0.394%
5	6.157	653	658	665	rBV	179448	199703	6.46%	1.122%
6	6.410	698	701	704	rBV2	32308	43226	1.40%	0.243%
7	6.540	719	723	726	rBV	1281728	1092201	35.31%	6.138%
8	6.740	753	757	760	rBV	77186	65502	2.12%	0.368%
9	6.916	783	787	790	rVB	721184	574367	18.57%	3.228%
10	6.969	790	796	800	rBV	33276	33247	1.07%	0.187%
11	7.051	807	810	820	rVB	78365	83217	2.69%	0.468%
12	7.240	838	842	847	rVB	56381	53151	1.72%	0.299%
13	7.481	878	883	885	rBV	1431452	1262456	40.81%	7.095%
14	7.498	885	886	890	rVB	85523	44488	1.44%	0.250%
15	8.092	979	987	991	rBV	790128	715831	23.14%	4.023%
16	8.169	997	1000	1002	rBV	38351	33539	1.08%	0.188%
17	8.198	1002	1005	1008	rVV	881016	676823	21.88%	3.804%
18	8.245	1011	1013	1017	rBV3	41109	53712	1.74%	0.302%
19	8.345	1026	1030	1037	rBV5	17790	38569	1.25%	0.217%
20	8.775	1101	1103	1108	rVB	64742	51167	1.65%	0.288%
21	8.910	1122	1126	1129	rVB2	37749	32908	1.06%	0.185%
22	9.275	1184	1188	1191	rVB	2668902	2063919	66.72%	11.600%
23	9.345	1196	1200	1203	rBV	83305	71567	2.31%	0.402%
24	9.610	1238	1245	1248	rBV4	25083	45299	1.46%	0.255%
25	9.875	1284	1290	1293	rBV2	100575	90185	2.92%	0.507%
26	9.957	1299	1304	1307	rBV	871184	682984	22.08%	3.839%
27	9.986	1307	1309	1313	rVB	35945	32608	1.05%	0.183%
28	10.163	1336	1339	1342	rVB2	32463	31320	1.01%	0.176%
29	10.198	1342	1345	1349	rBV3	24700	31359	1.01%	0.176%
30	10.375	1372	1375	1378	rVB	103780	81427	2.63%	0.458%
31	10.504	1394	1397	1404	rVB	32704	34759	1.12%	0.195%
32	10.592	1410	1412	1415	rVB	40550	35654	1.15%	0.200%
33	10.851	1453	1456	1464	rVB2	99896	154825	5.01%	0.870%
34	11.298	1529	1532	1534	rBV	100562	79132	2.56%	0.445%
35	11.328	1534	1537	1545	rVB2	45490	64324	2.08%	0.362%
36	11.451	1554	1558	1560	rBV	709756	610146	19.73%	3.429%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050322\
Data File : BF128057.D
Acq On : 03 May 2022 20:38
Operator : CG\JU
Sample : N2659-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
22L097-B

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-BF042222.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	11.475	1560	1562	1567	rVV	236719	195573	6.32%	1.099%
38	11.522	1568	1570	1573	rVB	40653	34033	1.10%	0.191%
39	11.728	1602	1605	1607	rBV	54606	46210	1.49%	0.260%
40	11.951	1640	1643	1646	rBV	31562	33364	1.08%	0.188%
41	12.063	1659	1662	1664	rBV2	35508	36487	1.18%	0.205%
42	12.133	1671	1674	1677	rBV	50334	38673	1.25%	0.217%
43	12.522	1738	1740	1742	rBV2	43399	42989	1.39%	0.242%
44	12.663	1761	1764	1768	rBV	257846	244927	7.92%	1.377%
45	12.898	1798	1804	1807	rBV	286325	300019	9.70%	1.686%
46	13.033	1823	1827	1831	rVB	1705183	1619728	52.36%	9.103%
47	13.251	1862	1864	1867	rBV2	39647	33188	1.07%	0.187%
48	13.504	1905	1907	1910	rVV	35992	33831	1.09%	0.190%
49	13.933	1977	1980	1989	rVB4	85573	191801	6.20%	1.078%
50	14.098	2004	2008	2010	rBV2	574690	562029	18.17%	3.159%
51	14.121	2010	2012	2018	rVB	104238	96457	3.12%	0.542%
52	15.604	2260	2264	2269	rBV	306595	396444	12.82%	2.228%

Sum of corrected areas: 17792985

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Instrument :
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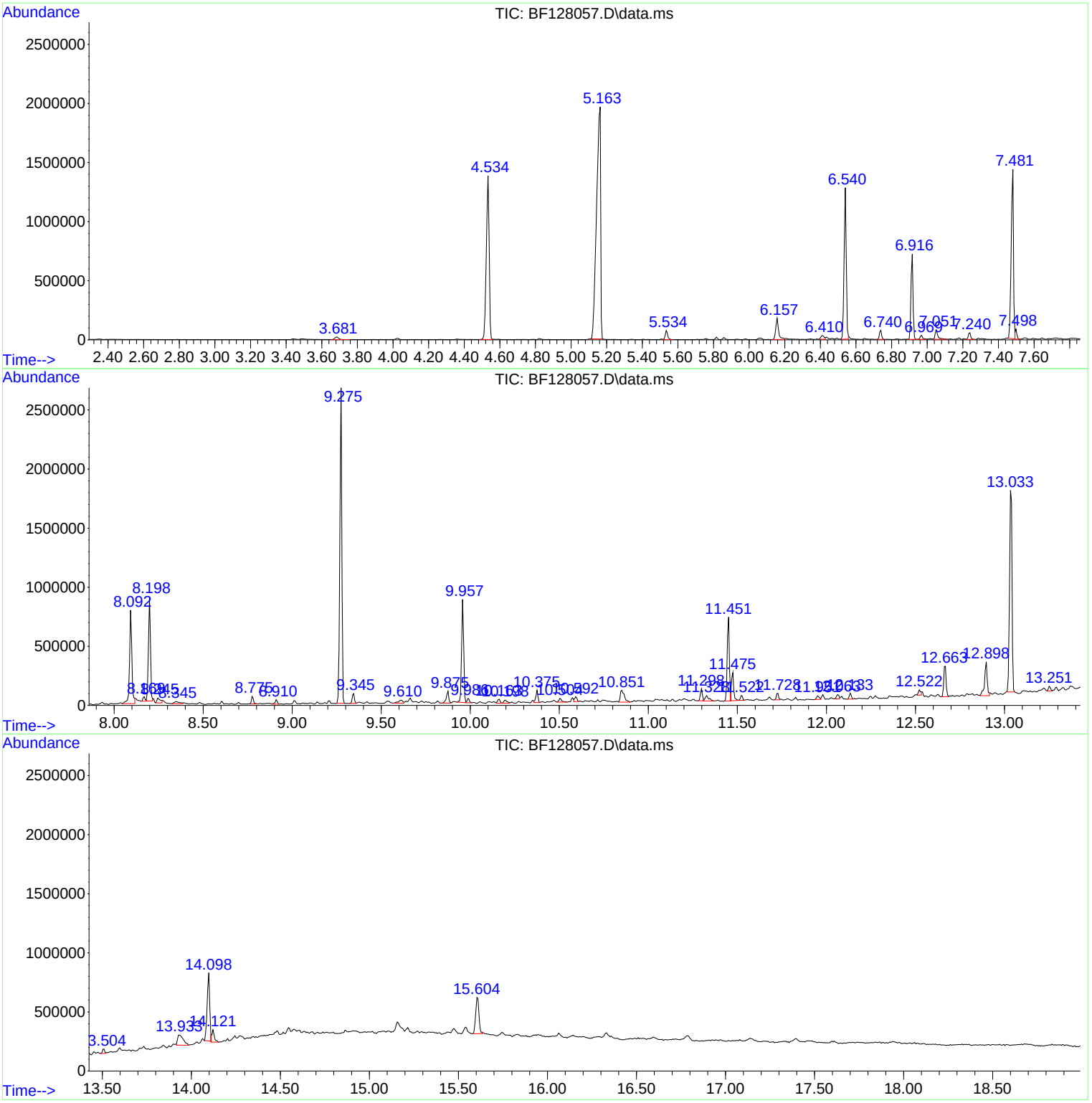
ClientSampleId :
22L097-B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.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\BF050322\
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Operator : CG\JU
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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

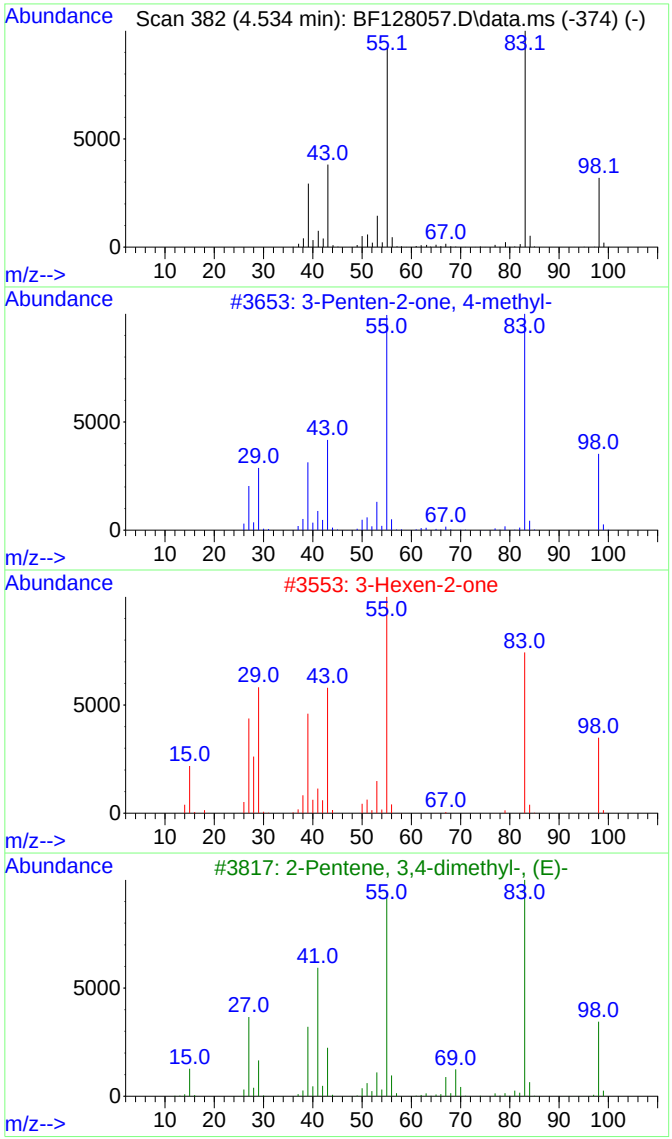
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

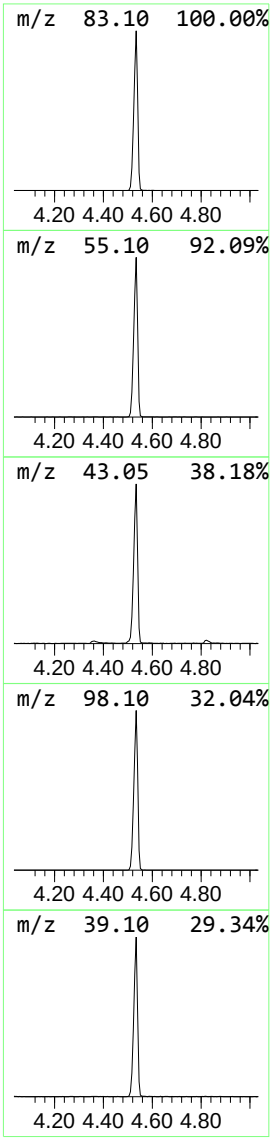
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.534	53.18 ng	1527150	1,4-Dichlorobenzene-d4	6.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86





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Operator : CG\JU
Sample : N2659-02
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ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
22L097-B

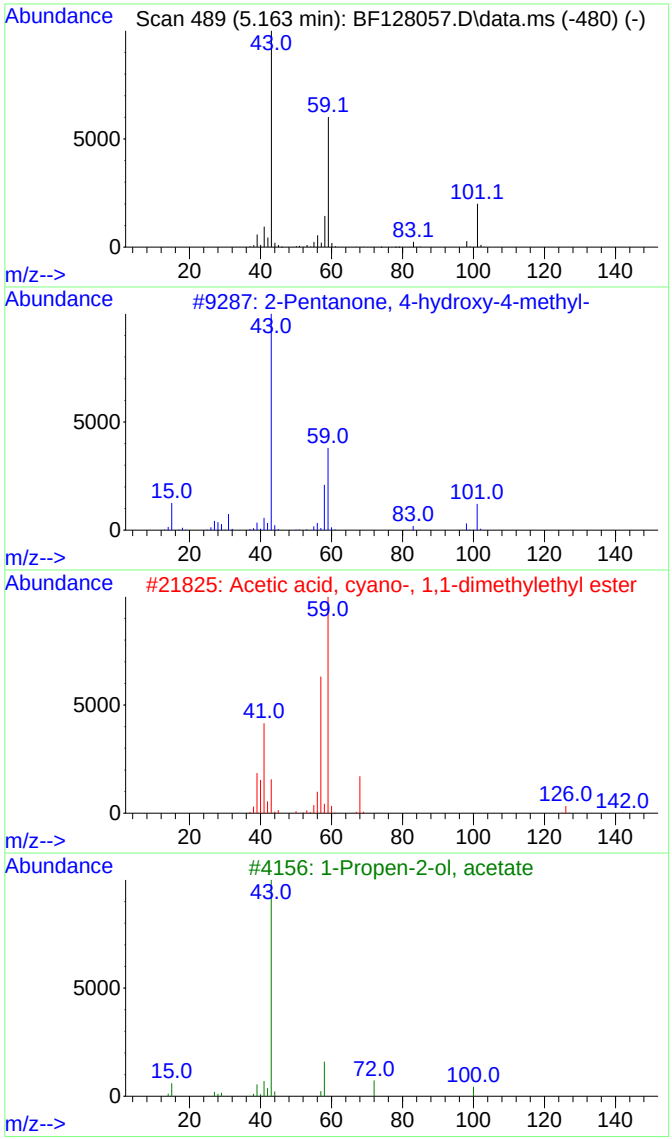
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

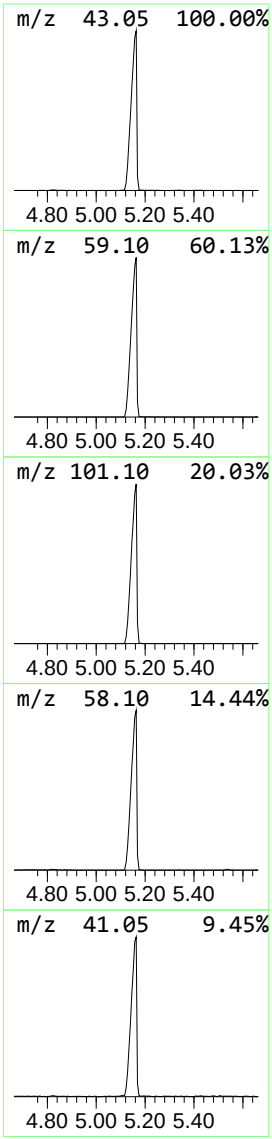
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.163	107.71 ng	3093170	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	72
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Operator : CG\JU
Sample : N2659-02
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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.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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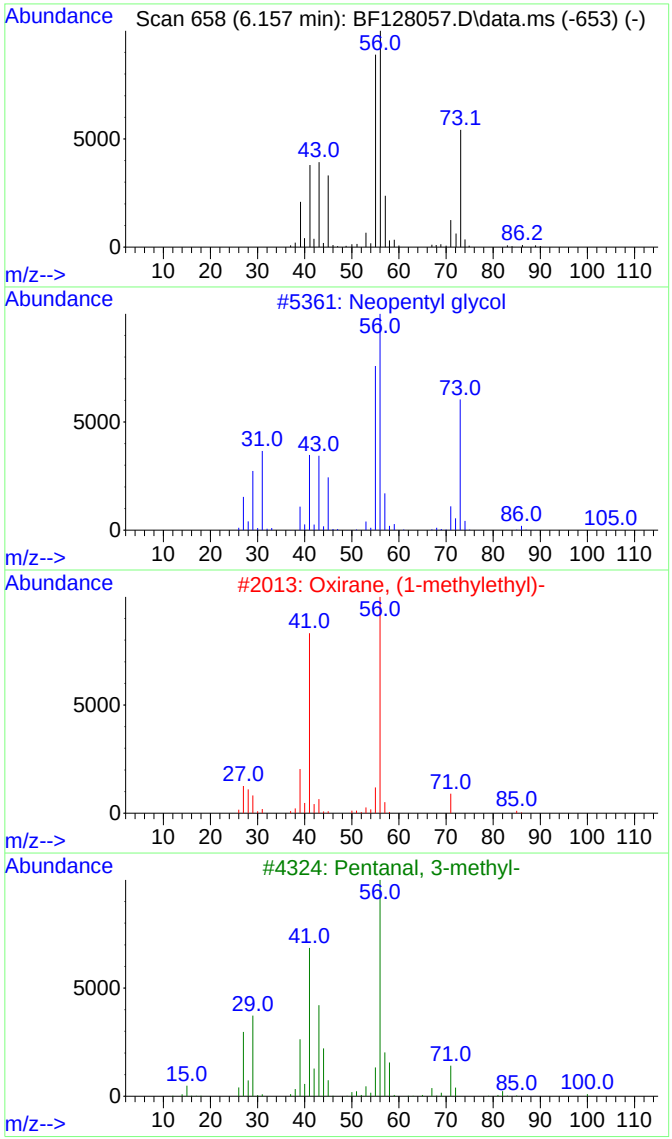
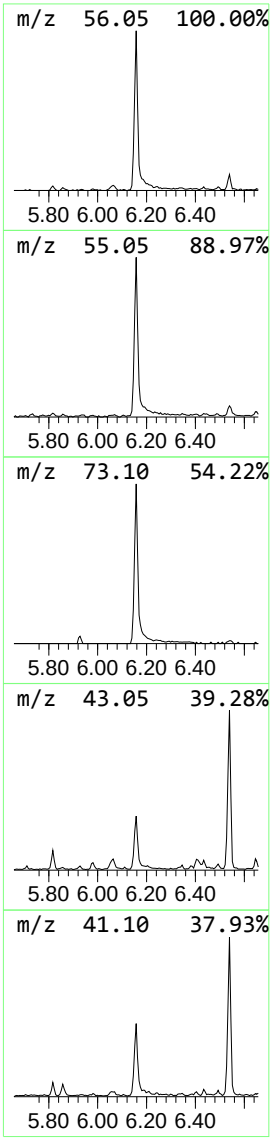
Peak Number 3 Neopentyl glycol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.157	6.95 ng	199703	1,4-Dichlorobenzene-d4	6.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Neopentyl glycol	104	C5H12O2	000126-30-7	83
2	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	47
3	Pentanal, 3-methyl-	100	C6H12O	015877-57-3	40
4	2,4-Pentanediol, 3-methyl-	118	C6H14O2	005683-44-3	38
5	4-Heptanol	116	C7H16O	000589-55-9	12





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Sample : N2659-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
22L097-B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.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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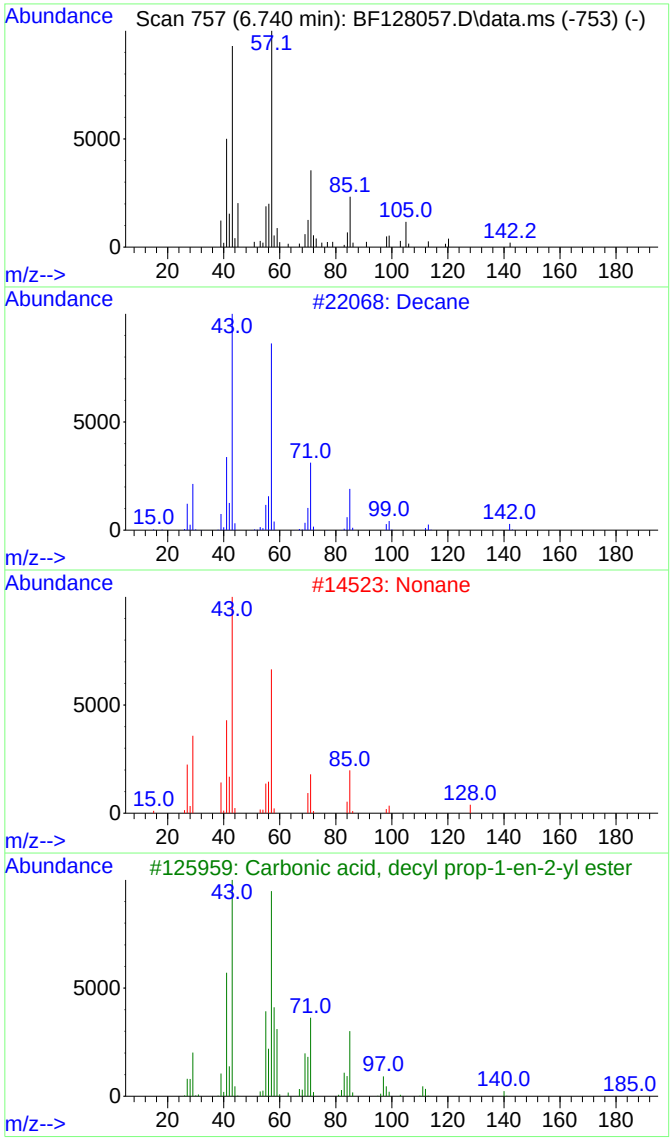
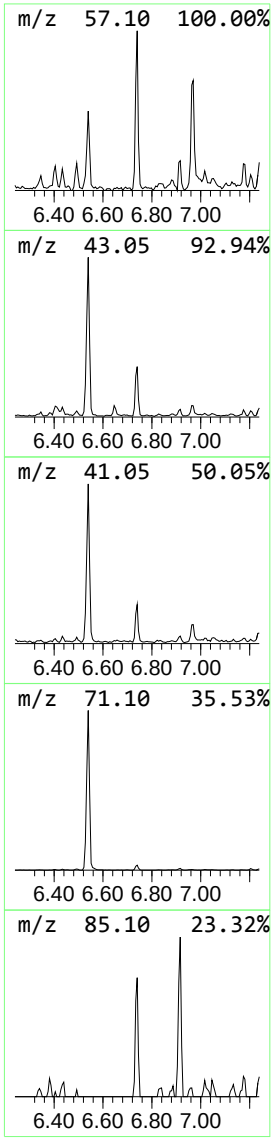
Peak Number 4 Decane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.740	2.28 ng	65502	1,4-Dichlorobenzene-d4	6.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane	142	C10H22	000124-18-5	58
2	Nonane	128	C9H20	000111-84-2	58
3	Carbonic acid, decyl prop-1-en-2...	242	C14H26O3	1000382-90-5	53
4	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	50
5	Tridecane	184	C13H28	000629-50-5	50





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Sample : N2659-02
Misc :
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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.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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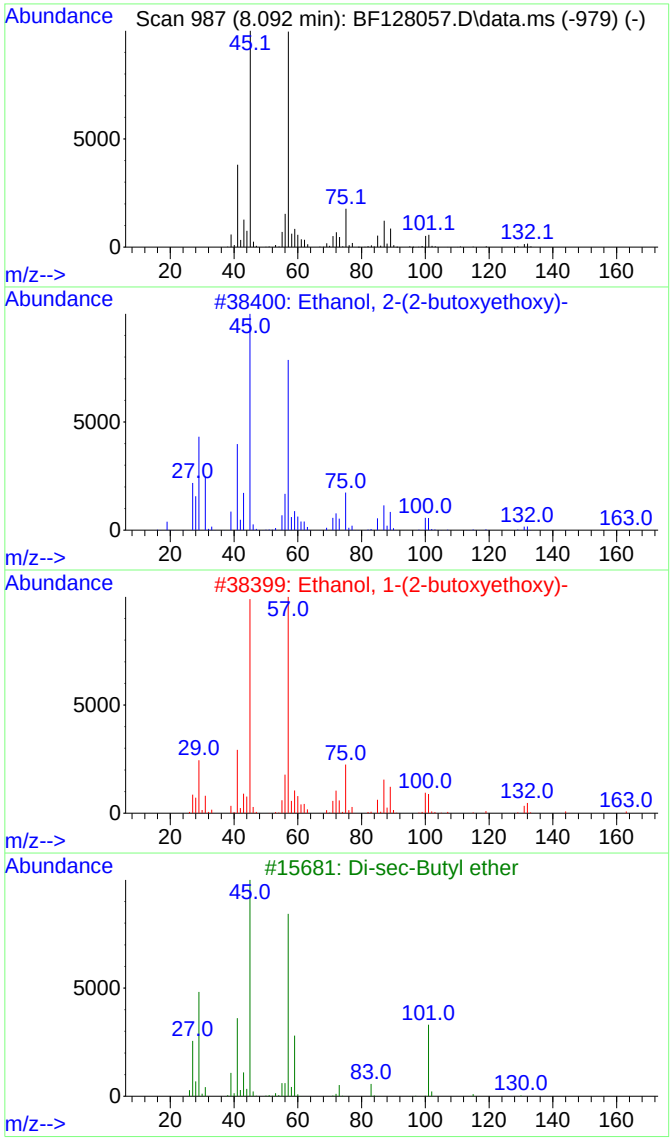
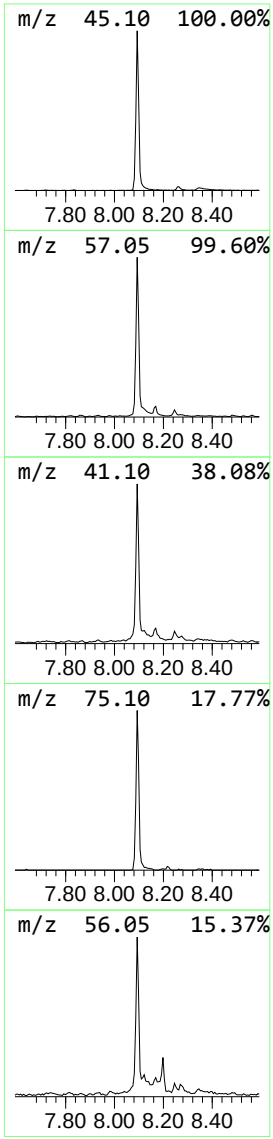
Peak Number 5 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.092	21.15 ng	715831	Naphthalene-d8	8.198

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
3	Di-sec-Butyl ether	130	C8H18O	006863-58-7	59
4	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
5	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50





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ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.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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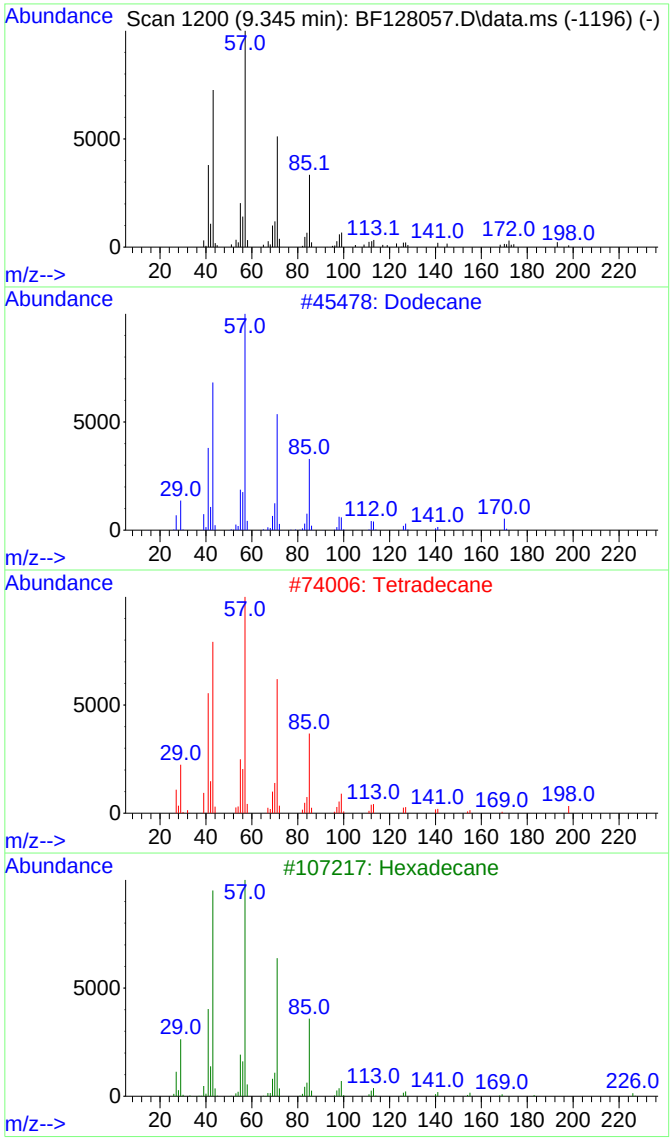
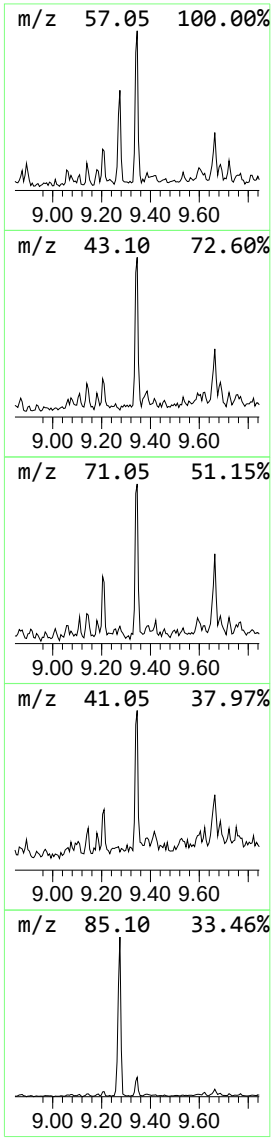
Peak Number 6 Dodecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.345	2.10 ng	71567	Acenaphthene-d10	9.957

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	93
2	Tetradecane	198	C14H30	000629-59-4	91
3	Hexadecane	226	C16H34	000544-76-3	91
4	Decane, 3,6-dimethyl-	170	C12H26	017312-53-7	86
5	Tridecane	184	C13H28	000629-50-5	86





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Acq On : 03 May 2022 20:38
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Sample : N2659-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
22L097-B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.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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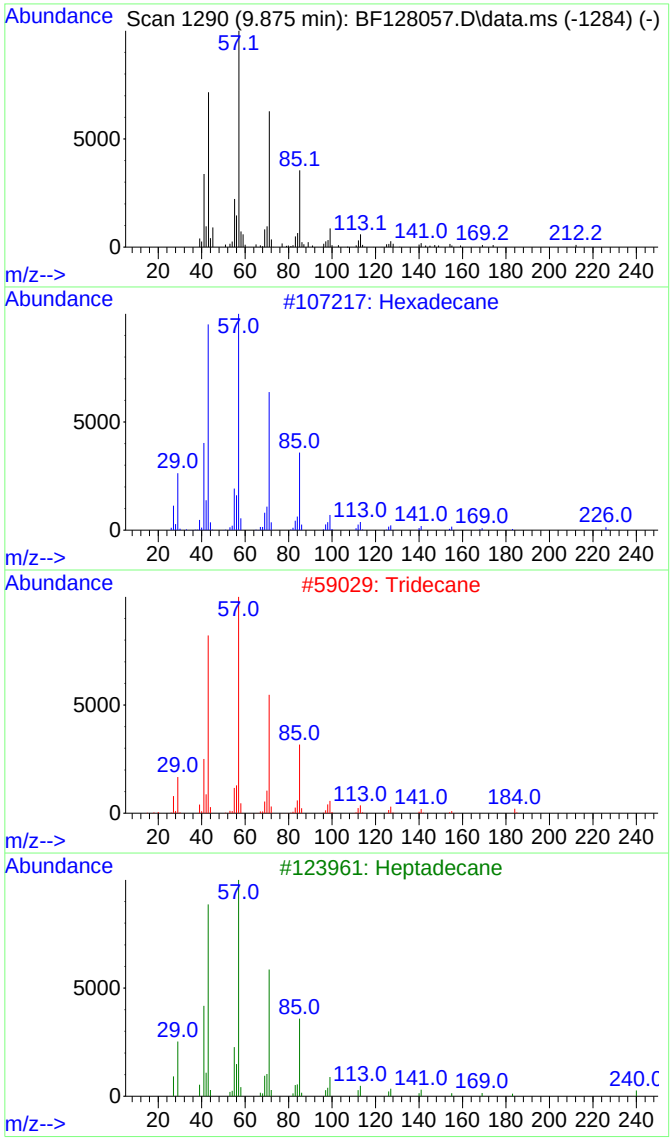
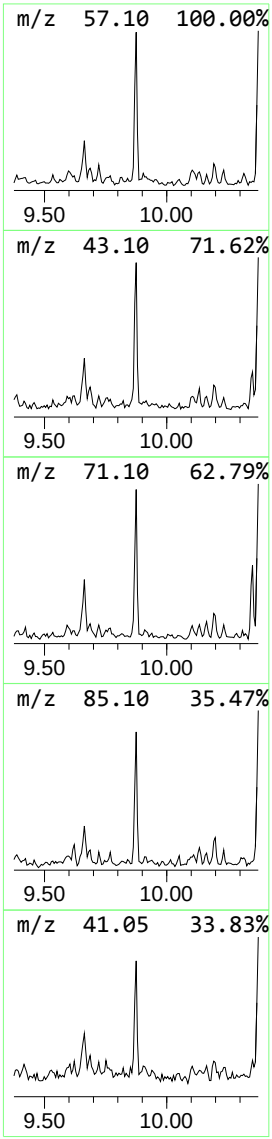
Peak Number 7 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.875	2.64 ng	90185	Acenaphthene-d10	9.957

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	86
2	Tridecane	184	C13H28	000629-50-5	86
3	Heptadecane	240	C17H36	000629-78-7	86
4	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	86
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050322\
Data File : BF128057.D
Acq On : 03 May 2022 20:38
Operator : CG\JU
Sample : N2659-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
22L097-B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.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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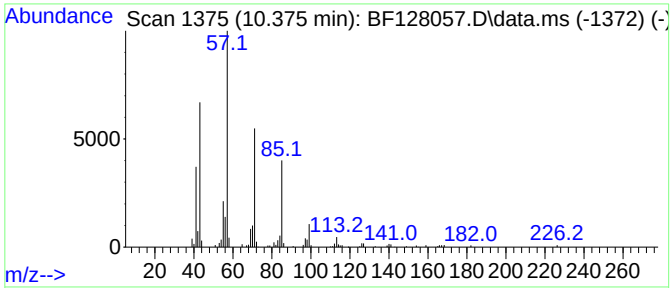
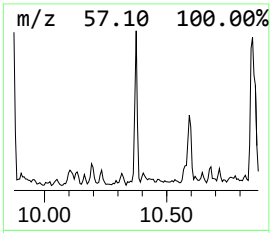
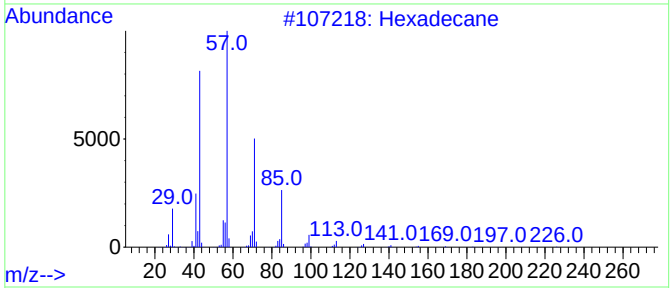
Peak Number 8 Nonadecane Concentration Rank 9

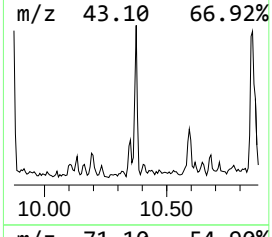
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.375	2.38 ng	81427	Acenaphthene-d10	9.957

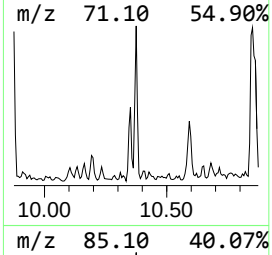
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	94
2	Nonadecane	268	C19H40	000629-92-5	91
3	Pentadecane	212	C15H32	000629-62-9	90
4	Heptacosane	380	C27H56	000593-49-7	90
5	Heptadecane	240	C17H36	000629-78-7	90

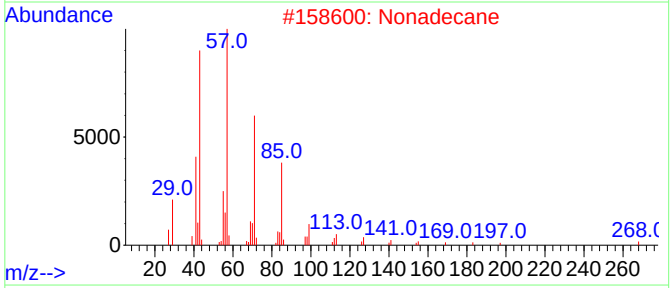


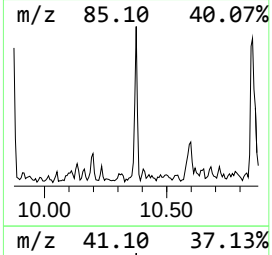


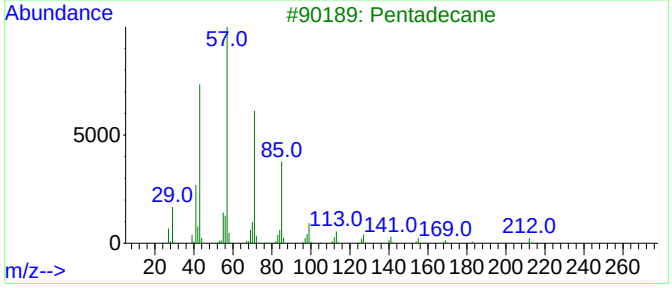


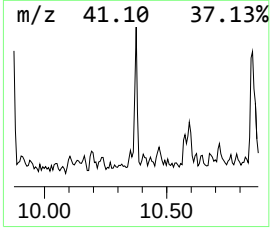












Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050322\
Data File : BF128057.D
Acq On : 03 May 2022 20:38
Operator : CG\JU
Sample : N2659-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
22L097-B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.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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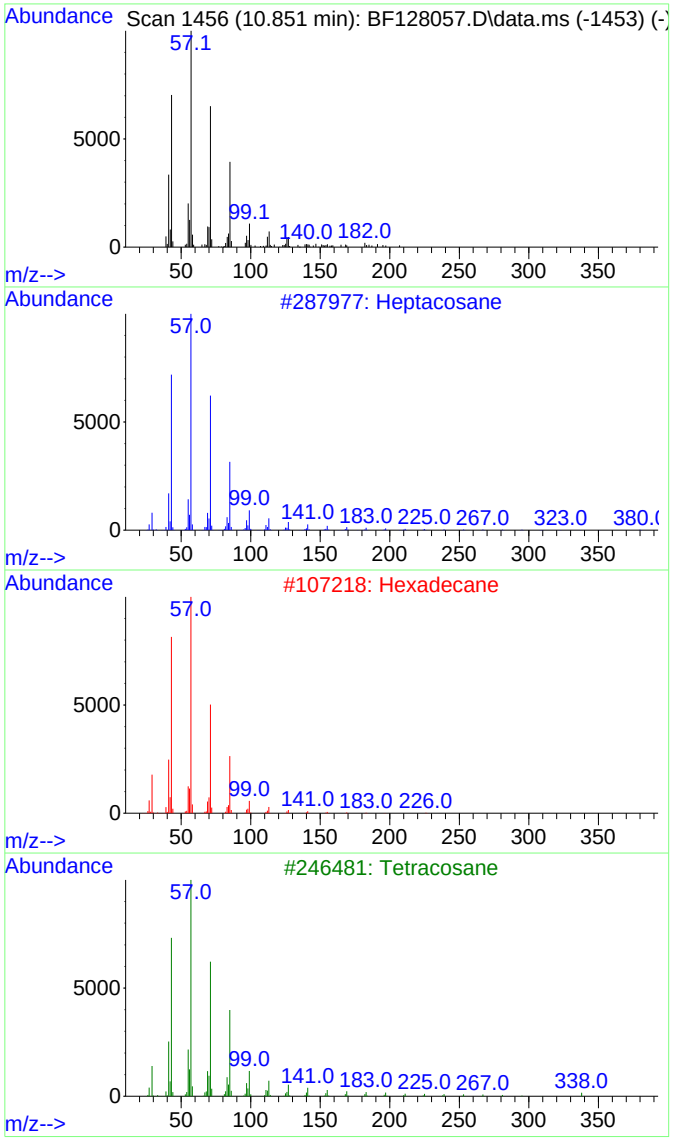
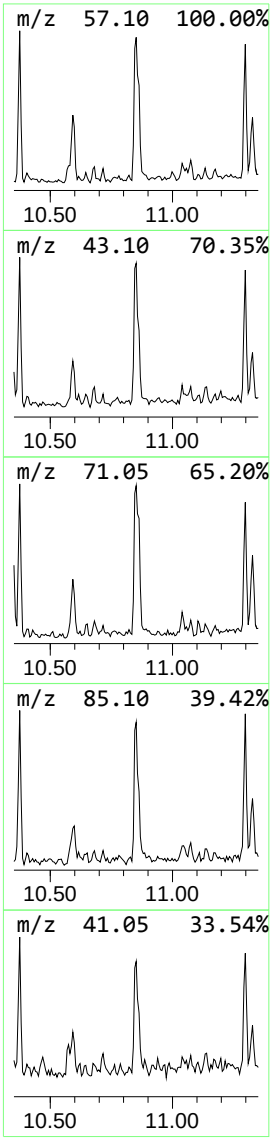
Peak Number 9 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.851	5.08 ng	154825	Phenanthrene-d10	11.451

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	90
2	Hexadecane	226	C16H34	000544-76-3	90
3	Tetracosane	338	C24H50	000646-31-1	87
4	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	86
5	Tetradecane	198	C14H30	000629-59-4	86





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Acq On : 03 May 2022 20:38
Operator : CG\JU
Sample : N2659-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
22L097-B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.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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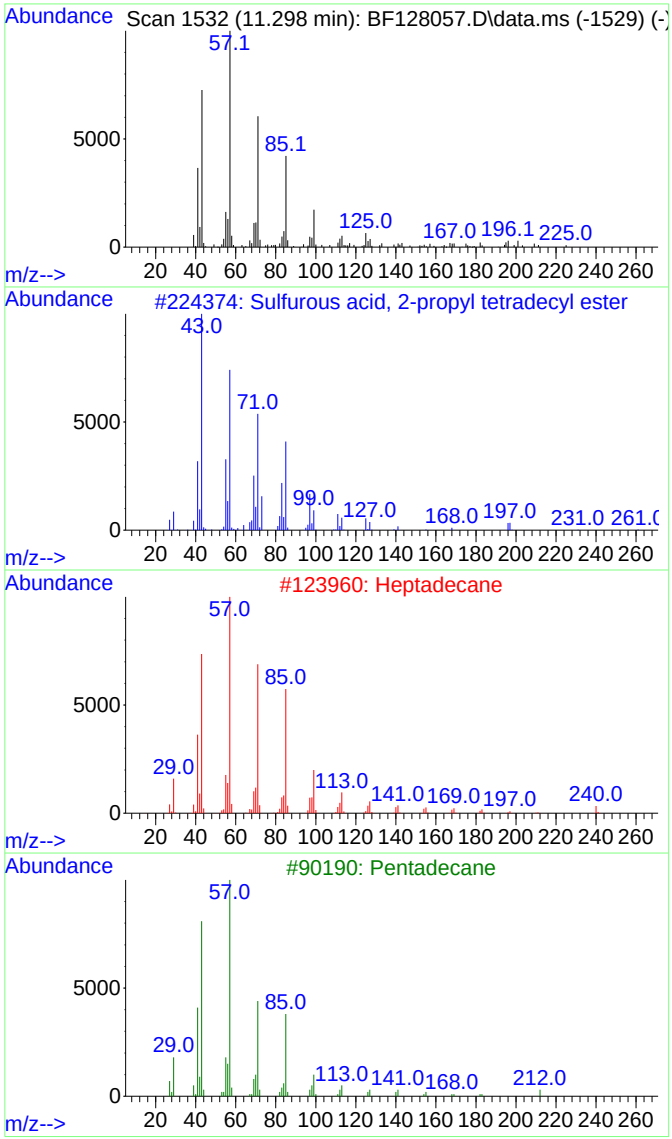
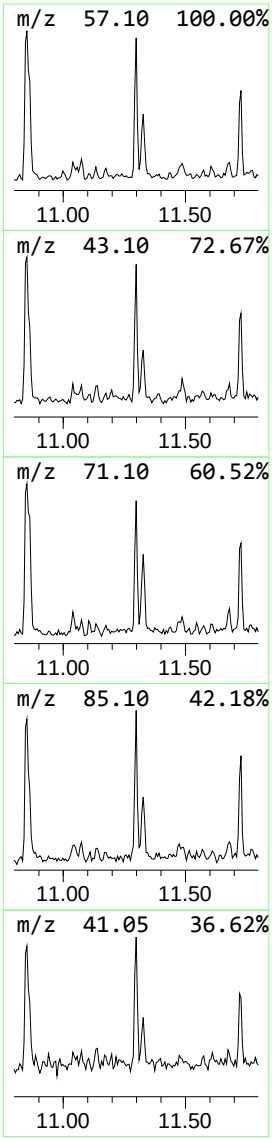
Peak Number 10 Sulfurous acid, 2-propyl te... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.298	2.59 ng	79132	Phenanthrene-d10	11.451

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, 2-propyl tetrade...	320	C17H36O3S	1010309-12-5	91
2	Heptadecane	240	C17H36	000629-78-7	86
3	Pentadecane	212	C15H32	000629-62-9	86
4	Tetracosane	338	C24H50	000646-31-1	83
5	Eicosane	282	C20H42	000112-95-8	80





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Data File : BF128057.D
Acq On : 03 May 2022 20:38
Operator : CG\JU
Sample : N2659-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
22L097-B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.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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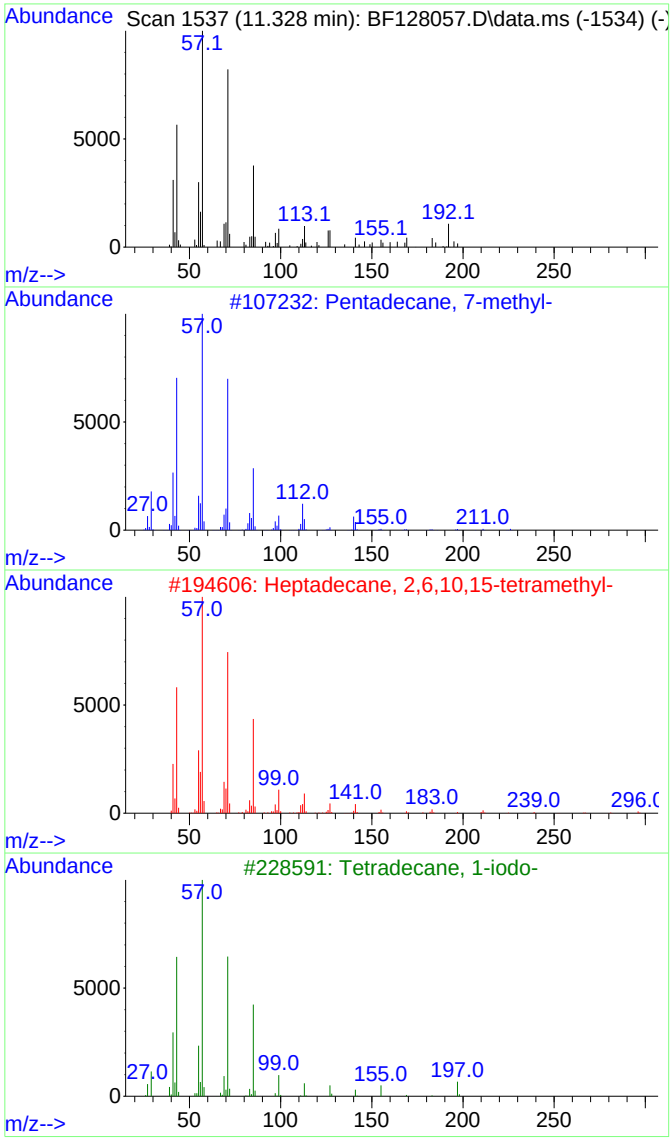
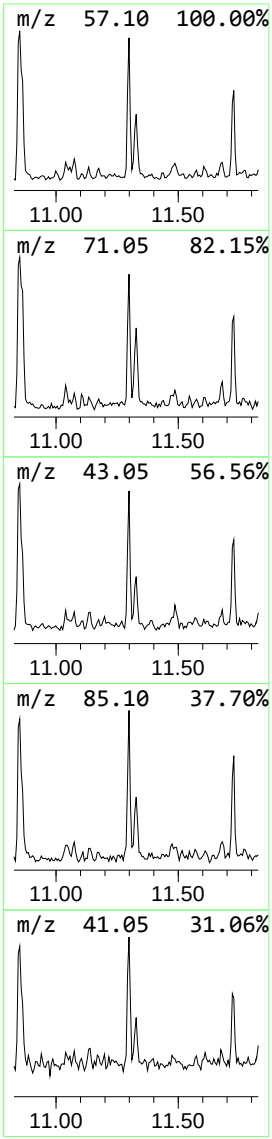
Peak Number 11 Pentadecane, 7-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.328	2.11 ng	64324	Phenanthrene-d10	11.451

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 7-methyl-	226	C16H34	006165-40-8	80
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	80
3	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	80
4	Hexadecane, 7,9-dimethyl-	254	C18H38	021164-95-4	80
5	Heneicosane	296	C21H44	000629-94-7	78





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050322\
Data File : BF128057.D
Acq On : 03 May 2022 20:38
Operator : CG\JU
Sample : N2659-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
22L097-B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.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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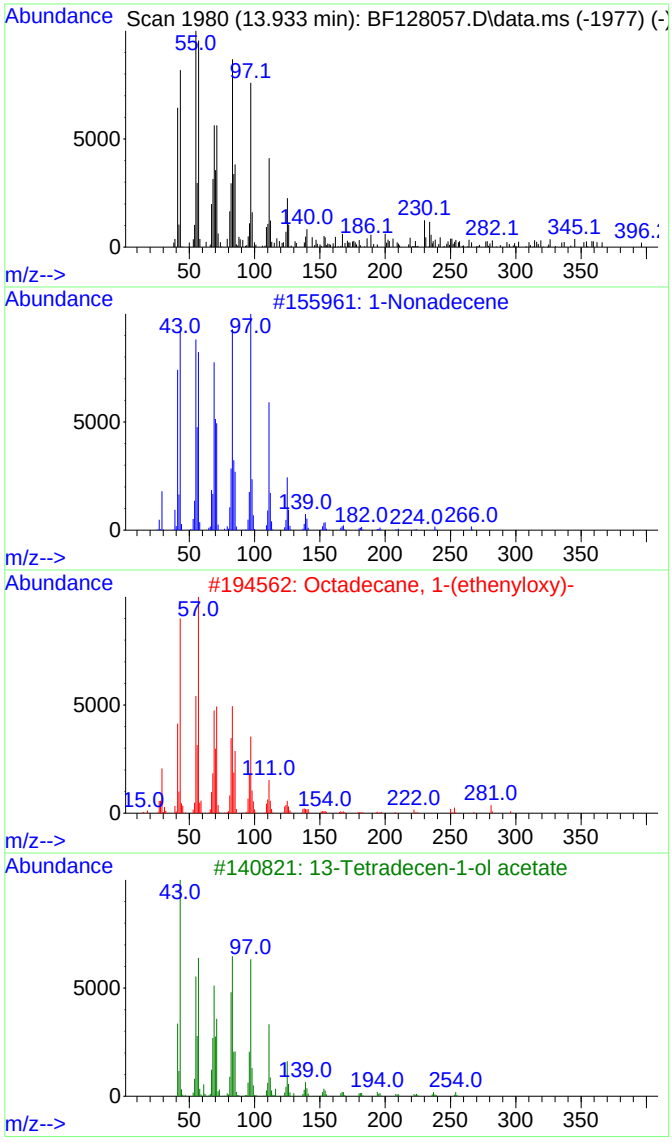
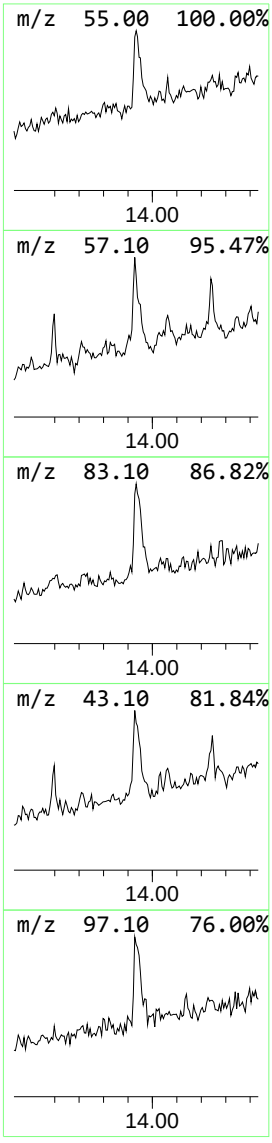
Peak Number 12 1-Nonadecene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.933	6.83 ng	191801	Chrysene-d12	14.098

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	96
2	Octadecane, 1-(ethenyloxy)-	296	C20H40O	000930-02-9	93
3	13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	91
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	90
5	Behenic alcohol	326	C22H46O	000661-19-8	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050322\
Data File : BF128057.D
Acq On : 03 May 2022 20:38
Operator : CG\JU
Sample : N2659-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
22L097-B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.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
3-Penten-2-one,...	4.534	53.2	ng	1527150	1	6.916	574367	20.0
2-Pentanone, 4-...	5.163	107.7	ng	3093170	1	6.916	574367	20.0
Neopentyl glycol	6.157	7.0	ng	199703	1	6.916	574367	20.0
Decane	6.740	2.3	ng	65502	1	6.916	574367	20.0
Ethanol, 2-(2-b...	8.092	21.1	ng	715831	2	8.198	676823	20.0
Dodecane	9.345	2.1	ng	71567	3	9.957	682984	20.0
Hexadecane	9.875	2.6	ng	90185	3	9.957	682984	20.0
Nonadecane	10.375	2.4	ng	81427	3	9.957	682984	20.0
Heptacosane	10.851	5.1	ng	154825	4	11.451	610146	20.0
Sulfurous acid,...	11.298	2.6	ng	79132	4	11.451	610146	20.0
Pentadecane, 7-...	11.328	2.1	ng	64324	4	11.451	610146	20.0
1-Nonadecene	13.933	6.8	ng	191801	5	14.098	562029	20.0