LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091521\
Data File : BF125524.D
Acq On : 16 Sep 2021 1:56
Operator : JU/CG
Sample : M3687-21 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A005015

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-BF091521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125524.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	3	8	14	rBV	510248	629972	26.79%	2.673%
2	2.269	29	31	38	rVB	25628	35359	1.50%	0.150%
3	4.463	391	404	405	rBV5	32799	87568	3.72%	0.372%
4	4.622	429	431	433	rVB	98878	70186	2.99%	0.298%
5	4.969	486	490	498	rBV	78156	89997	3.83%	0.382%
6	5.075	504	508	516	rBV	286859	314516	13.38%	1.335%
7	5.487	574	578	586	rBV	1717755	1549487	65.90%	6.576%
8	5.875	641	644	653	rVB2	33079	38527	1.64%	0.164%
9	6.257	705	709	712	rBV4	22093	33537	1.43%	0.142%
10	6.387	728	731	734	rVB	30629	30821	1.31%	0.131%
11	6.498	746	750	755	rBV	1599770	1611105	68.52%	6.837%
12	6.740	789	791	798	rVB3	27890	33672	1.43%	0.143%
13	6.863	809	812	816	rBV	1056098	964767	41.03%	4.094%
14	7.251	874	878	880	rBV	57016	68938	2.93%	0.293%
15	7.428	904	908	911	rBV	1138285	959840	40.82%	4.073%
16	7.545	925	928	938	rBV	91297	123668	5.26%	0.525%
17	7.951	984	997	1002	rBV2	619386	1545011	65.71%	6.557%
18	8.069	1013	1017	1023	rBV2	83985	156974	6.68%	0.666%
19	8.151	1027	1031	1033	rVV	1433601	1195412	50.84%	5.073%
20	8.169	1033	1034	1044	rVB	119040	126143	5.37%	0.535%
21	8.551	1086	1099	1102	rBV	1106891	2351131	100.00%	9.978%
22	8.957	1166	1168	1175	rBV2	46676	58207	2.48%	0.247%
23	9.104	1185	1193	1200	rBV	1191366	1891087	80.43%	8.025%
24	9.157	1200	1202	1207	rVV4	41691	52971	2.25%	0.225%
25	9.222	1209	1213	1217	rVB	1859038	1659949	70.60%	7.044%
26	9.328	1228	1231	1232	rBV	43454	41301	1.76%	0.175%
27	9.339	1232	1233	1236	rVB2	50657	36387	1.55%	0.154%
28	9.369	1236	1238	1245	rVB	92637	85625	3.64%	0.363%
29	9.439	1246	1250	1253	rVB5	25039	34480	1.47%	0.146%
30	9.492	1253	1259	1261	rBV7	18517	36511	1.55%	0.155%
31	9.616	1276	1280	1288	rBV	642656	695303	29.57%	2.951%
32	9.769	1302	1306	1308	rBV	53348	52041	2.21%	0.221%
33	9.828	1314	1316	1319	rVB	57928	43644	1.86%	0.185%
34	9.904	1326	1329	1333	rVB	1281389	1160866	49.37%	4.926%
35	10.116	1362	1365	1369	rBV2	65343	62349	2.65%	0.265%
36	10.328	1398	1401	1404	rVB2	68971	62142	2.64%	0.264%

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Misc :
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Instrument : BNA_F
ClientSampleId : A005015

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-BF091521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	10.698	1460	1464	1469	rBV	782671	772353	32.85%	3.278%
38	10.763	1473	1475	1479	rBV	75142	64917	2.76%	0.275%
39	10.804	1479	1482	1487	rBV	101140	126916	5.40%	0.539%
40	11.057	1523	1525	1528	rBV4	54712	63601	2.71%	0.270%
41	11.251	1556	1558	1560	rBV	81598	53568	2.28%	0.227%
42	11.398	1579	1583	1585	rBV	1156963	1005718	42.78%	4.268%
43	11.422	1585	1587	1590	rVB	156843	135852	5.78%	0.577%
44	11.927	1670	1673	1680	rVB	1101170	1117231	47.52%	4.741%
45	12.716	1804	1807	1810	rBV	768912	737334	31.36%	3.129%
46	12.986	1850	1853	1856	rVB	1143429	960409	40.85%	4.076%
47	14.051	2032	2034	2037	rVB	646986	536437	22.82%	2.277%

Sum of corrected areas: 23563830

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ClientSampleId :
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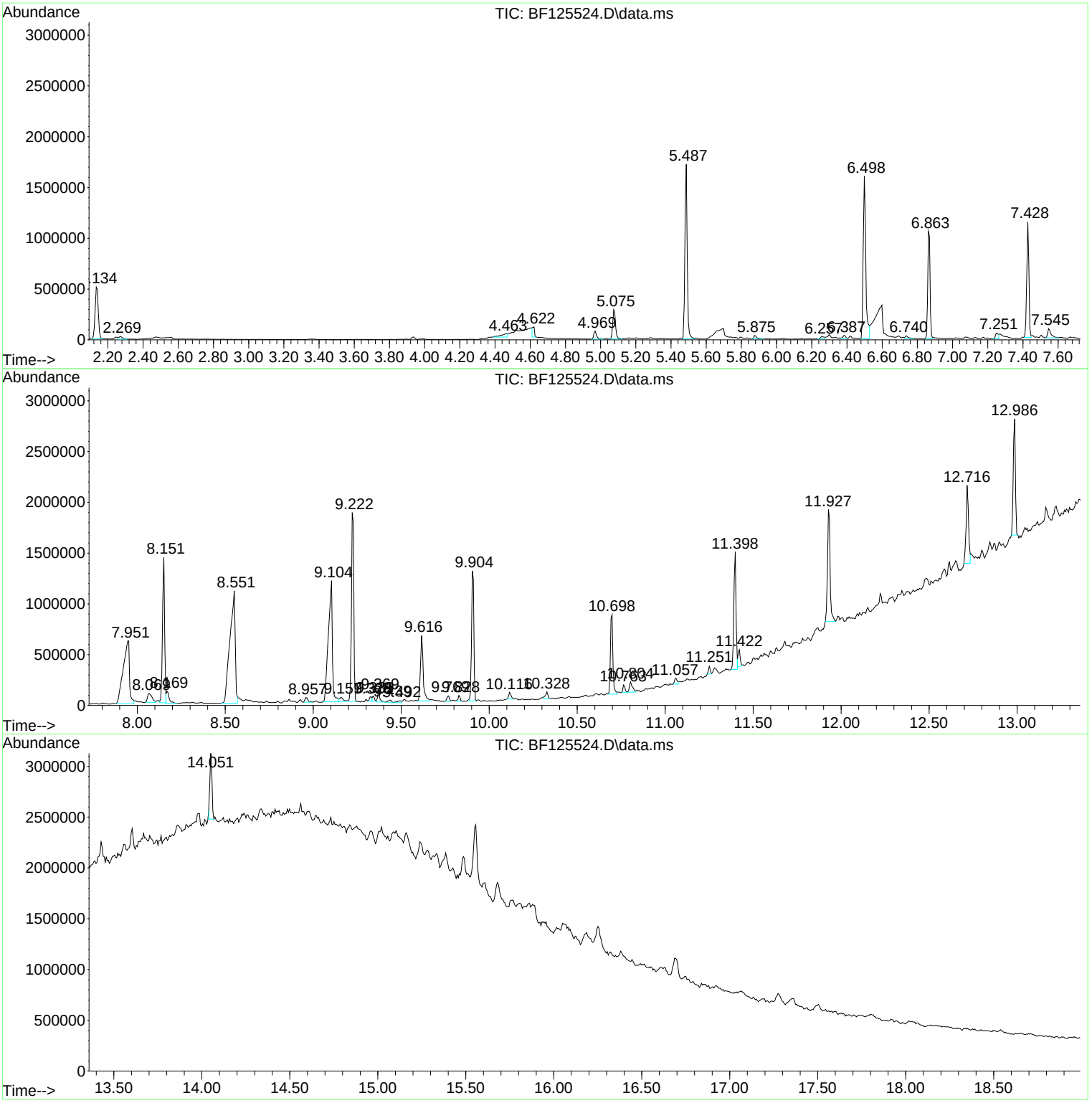
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091521\
Data File : BF125524.D
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Operator : JU/CG
Sample : M3687-21 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

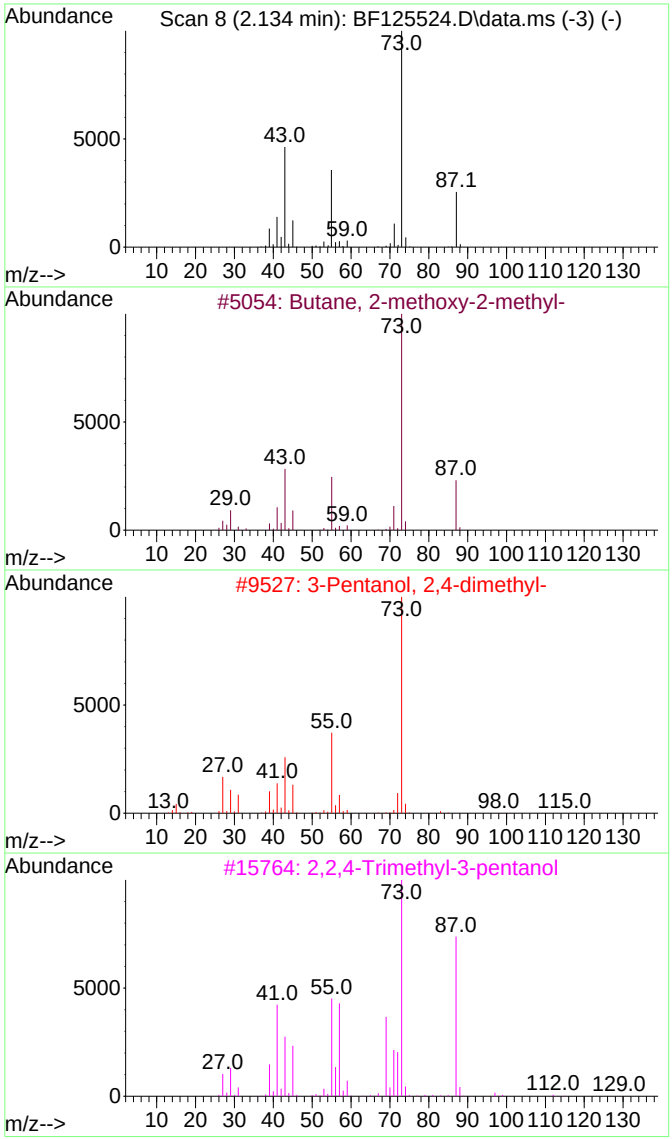
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

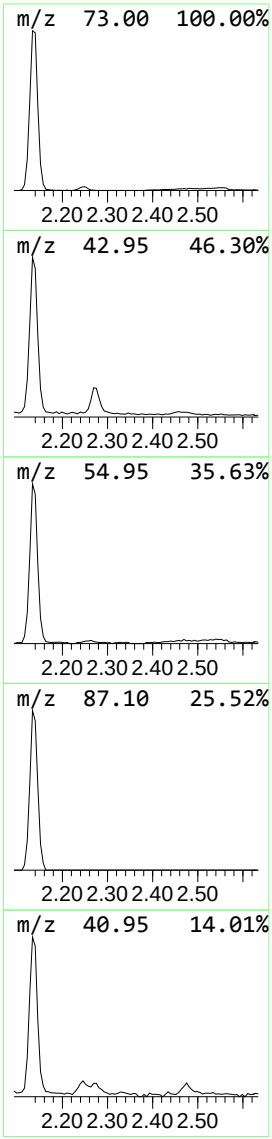
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.134	13.06 ng	629972	1,4-Dichlorobenzene-d4	6.869

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	39
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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Operator : JU/CG
Sample : M3687-21 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A005015

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091521.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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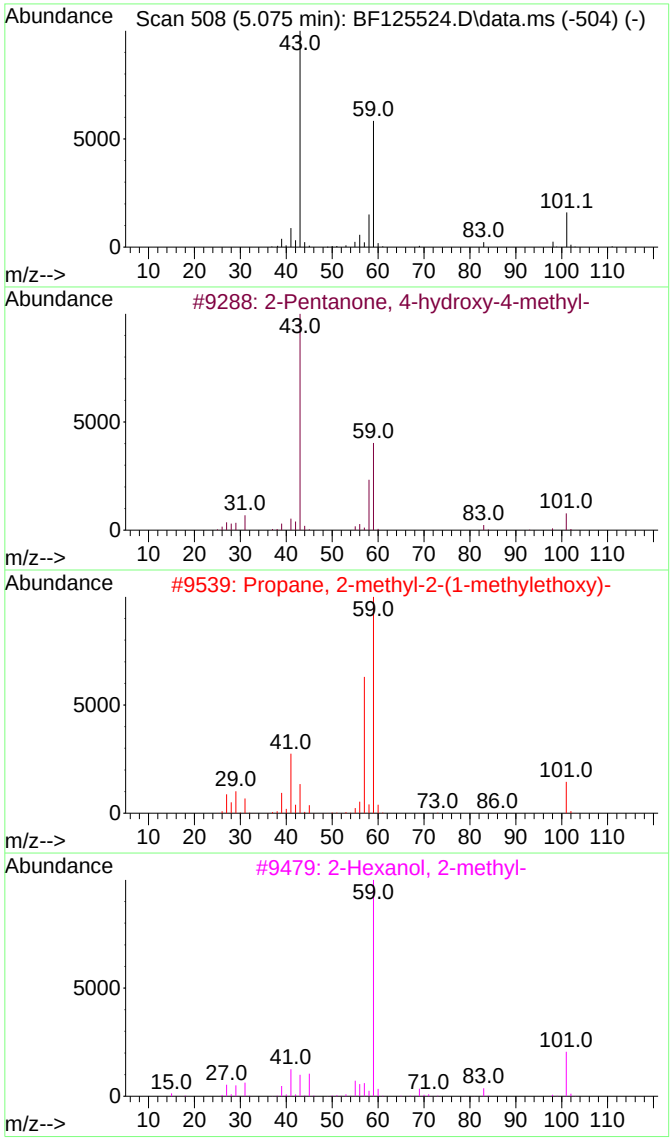
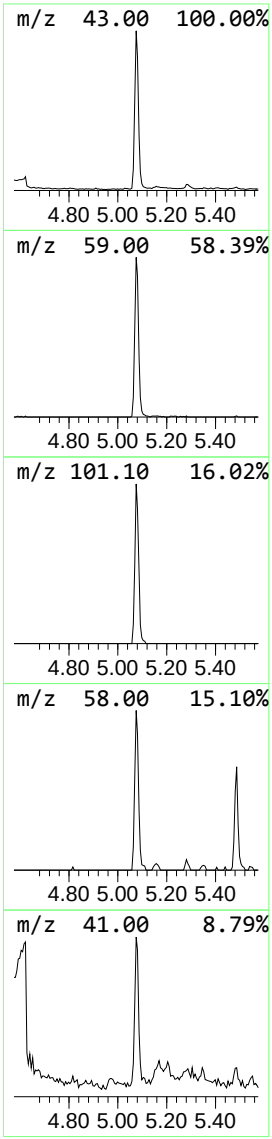
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	6.52 ng	314516	1,4-Dichlorobenzene-d4	6.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





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Sample : M3687-21 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A005015

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091521.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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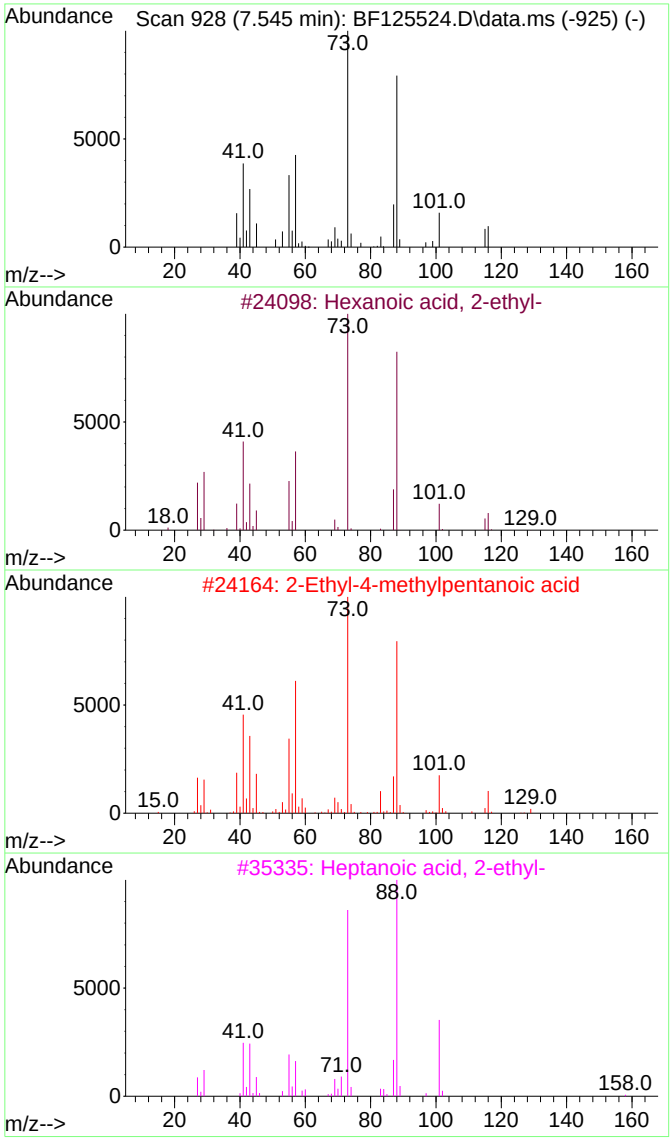
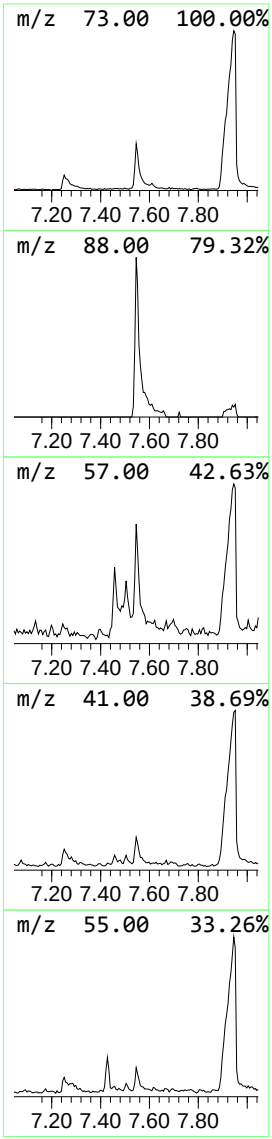
Peak Number 3 Hexanoic acid, 2-ethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.545	2.07 ng	123668	Naphthalene-d8	8.151

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	83
2	2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	64
3	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	53
4	Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	50
5	1,4-Dioxane	88	C4H8O2	000123-91-1	47





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Operator : JU/CG
Sample : M3687-21 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A005015

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091521.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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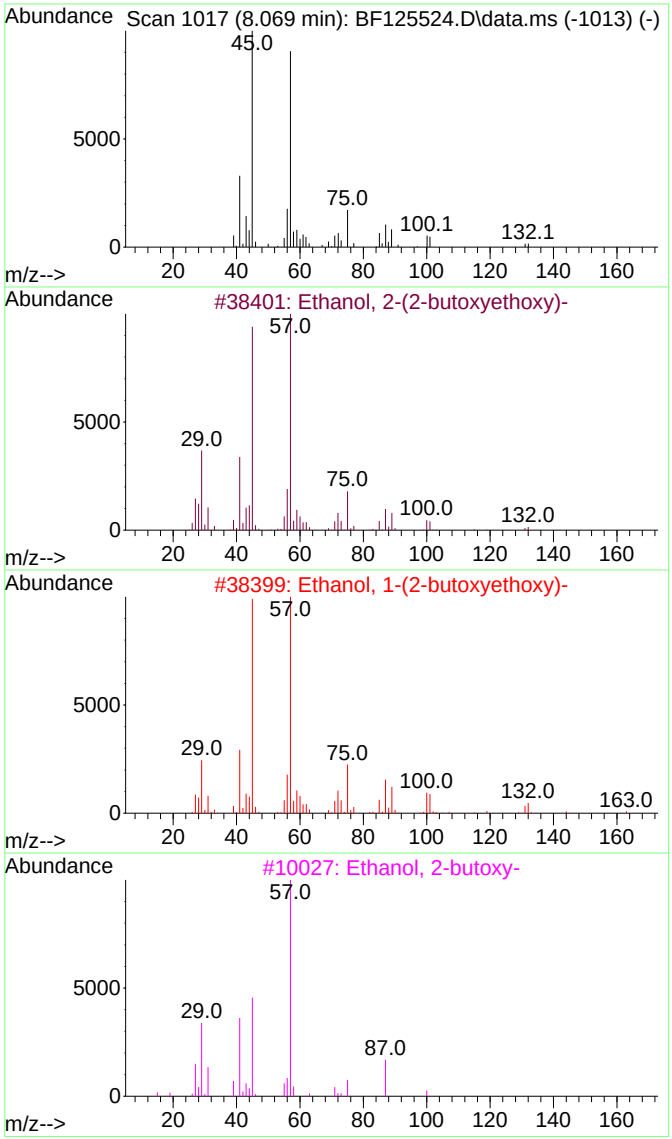
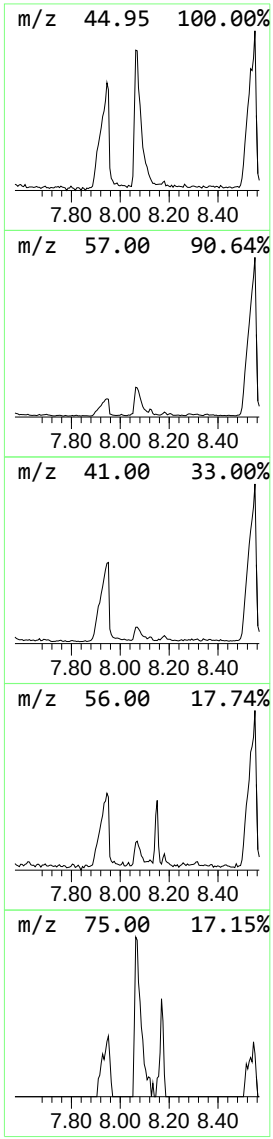
Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.069	2.63 ng	156974	Naphthalene-d8	8.151

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	83
3	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	50
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	50
5	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091521\
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Operator : JU/CG
Sample : M3687-21 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A005015

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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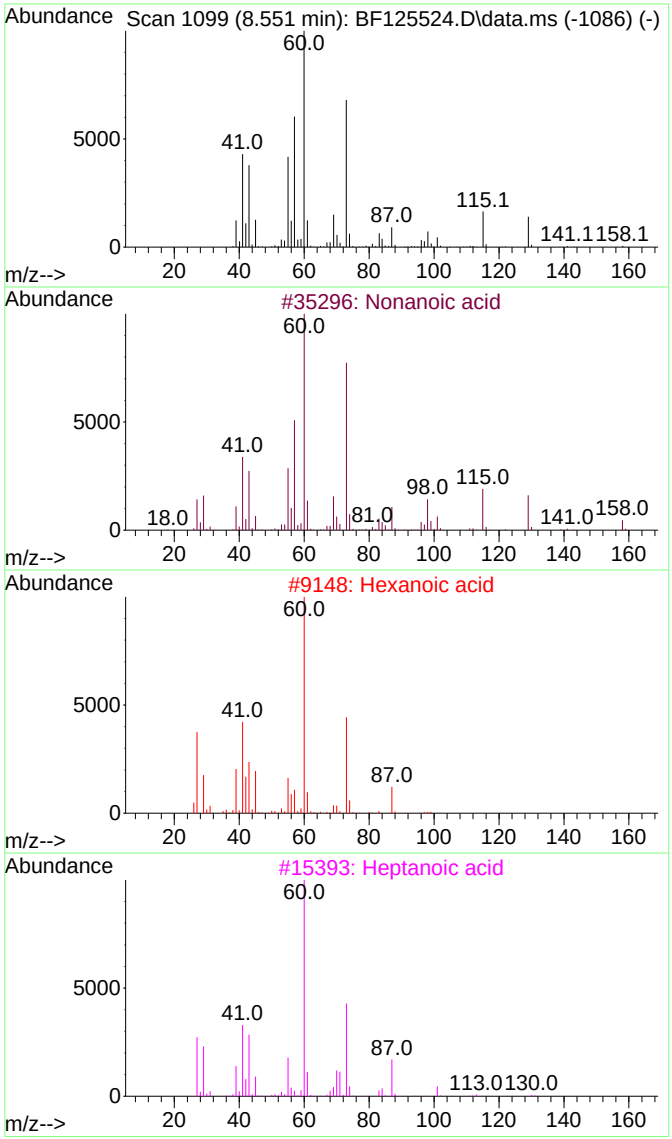
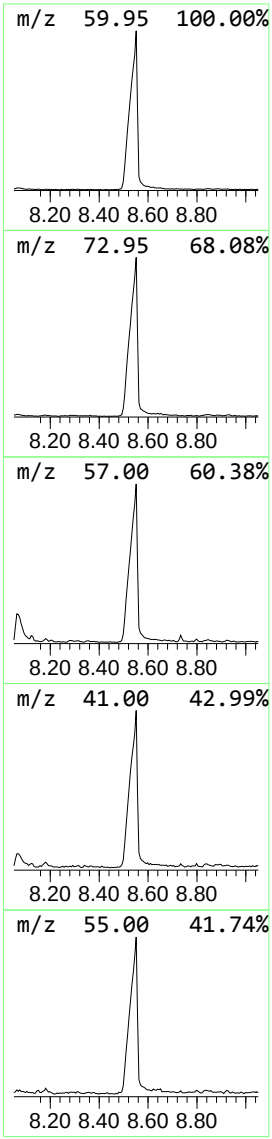
Peak Number 5 Nonanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.551	39.34 ng	2351130	Naphthalene-d8	8.151

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanoic acid	158	C9H18O2	000112-05-0	83
2	Hexanoic acid	116	C6H12O2	000142-62-1	64
3	Heptanoic acid	130	C7H14O2	000111-14-8	64
4	Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	59
5	Pentanoic acid	102	C5H10O2	000109-52-4	53





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Sample : M3687-21 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A005015

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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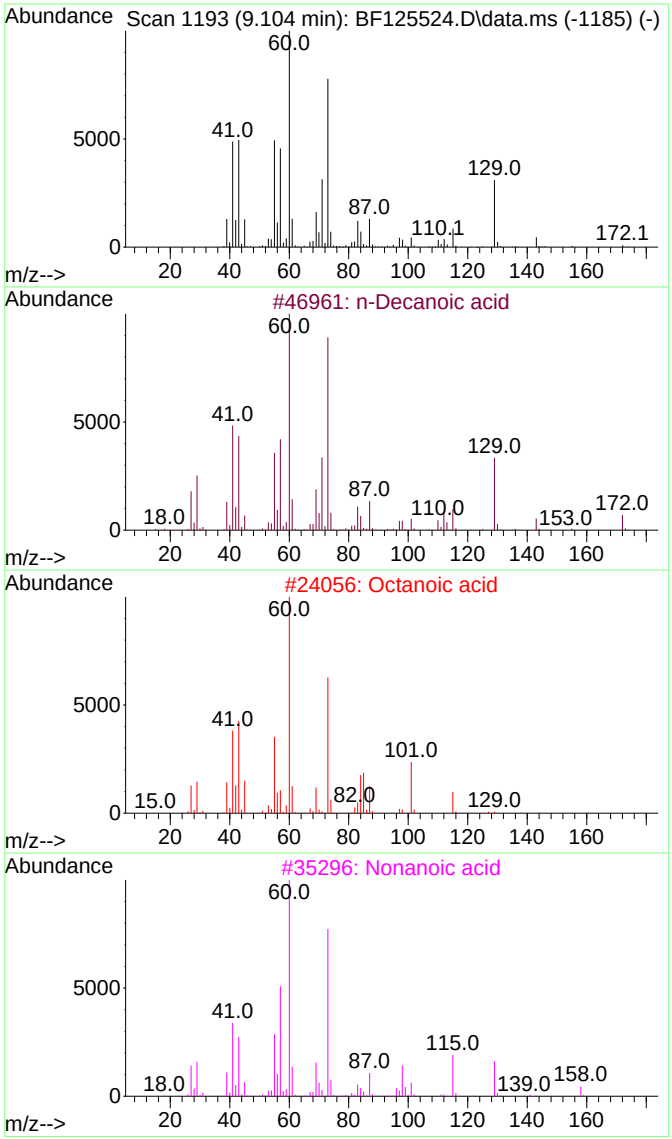
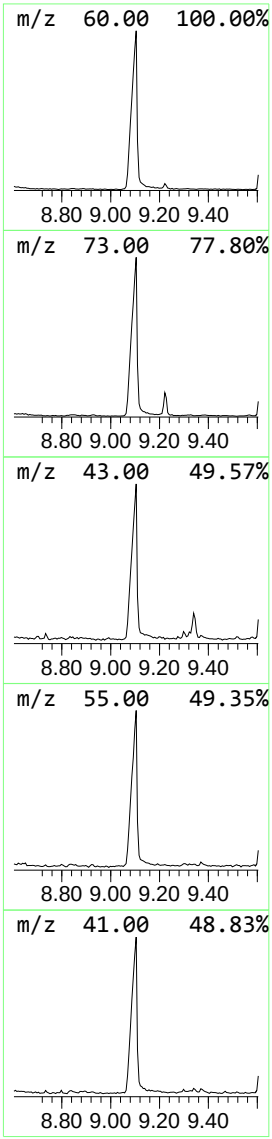
Peak Number 6 n-Decanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.104	32.58 ng	1891090	Acenaphthene-d10	9.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Decanoic acid	172	C10H20O2	000334-48-5	90
2	Octanoic acid	144	C8H16O2	000124-07-2	64
3	Nonanoic acid	158	C9H18O2	000112-05-0	59
4	Heptanoic acid	130	C7H14O2	000111-14-8	53
5	Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	52





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Misc :
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Instrument : BNA_F
ClientSampleId : A005015

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091521.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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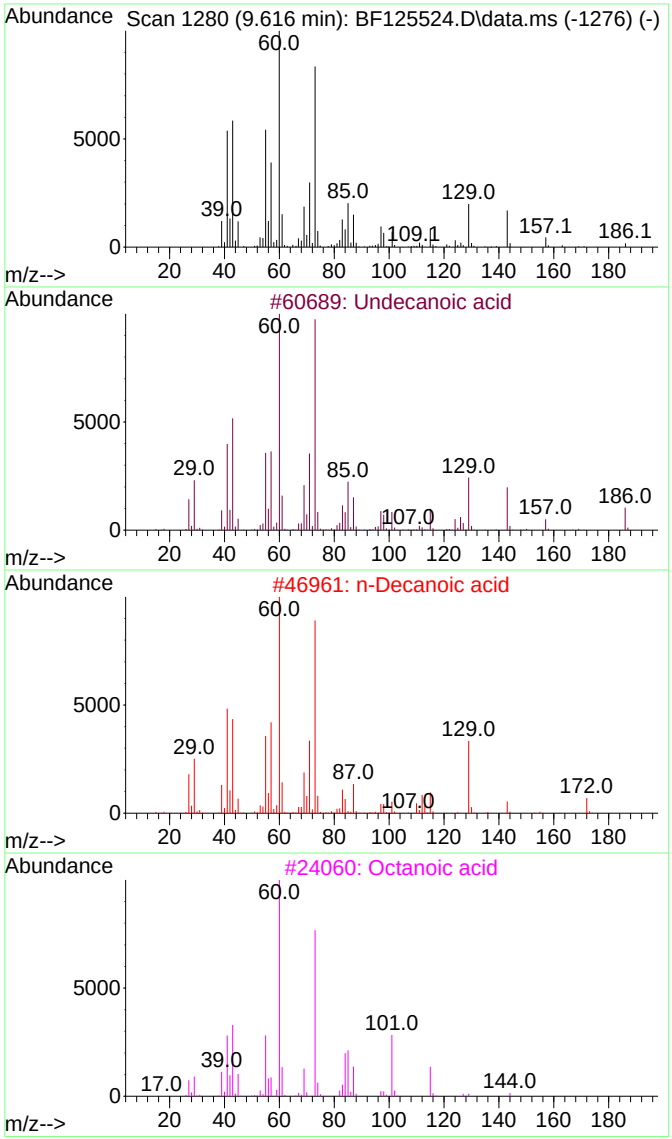
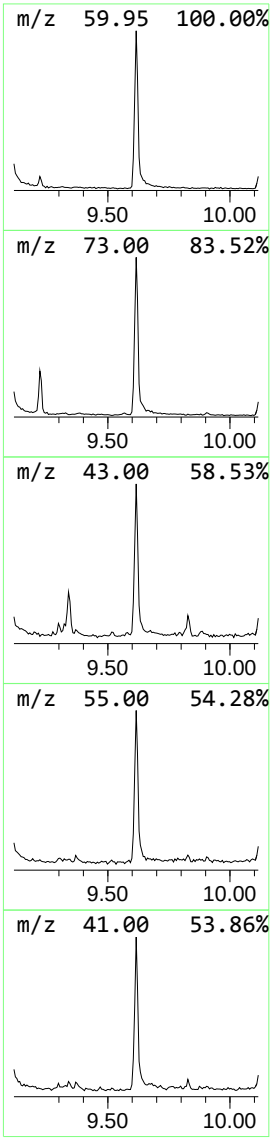
Peak Number 7 Undecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.616	11.98 ng	695303	Acenaphthene-d10	9.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	72
2	n-Decanoic acid	172	C10H20O2	000334-48-5	64
3	Octanoic acid	144	C8H16O2	000124-07-2	62
4	Nonanoic acid	158	C9H18O2	000112-05-0	52
5	Heptanoic acid	130	C7H14O2	000111-14-8	47





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Operator : JU/CG
Sample : M3687-21 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A005015

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091521.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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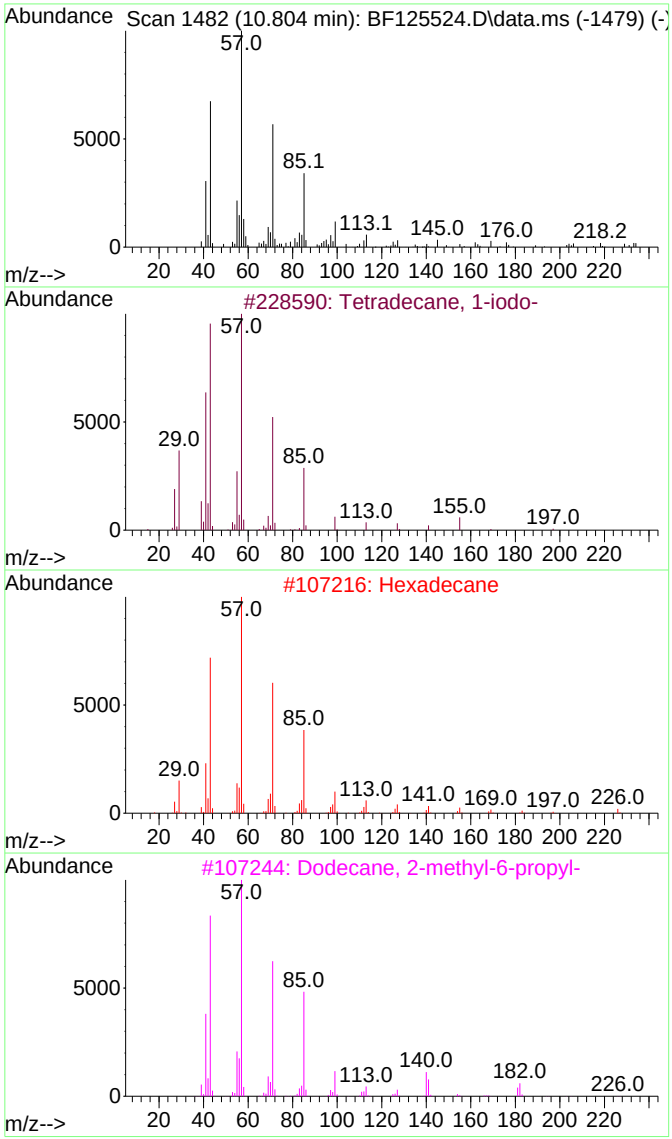
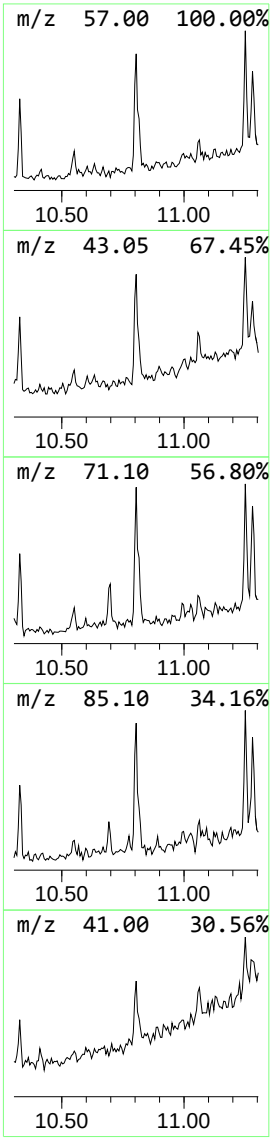
Peak Number 8 Tetradecane, 1-iodo- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.804	2.52 ng	126916	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	80
2	Hexadecane	226	C16H34	000544-76-3	80
3	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	80
4	Tetracosane	338	C24H50	000646-31-1	80
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	80





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Acq On : 16 Sep 2021 1:56
Operator : JU/CG
Sample : M3687-21 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A005015

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091521.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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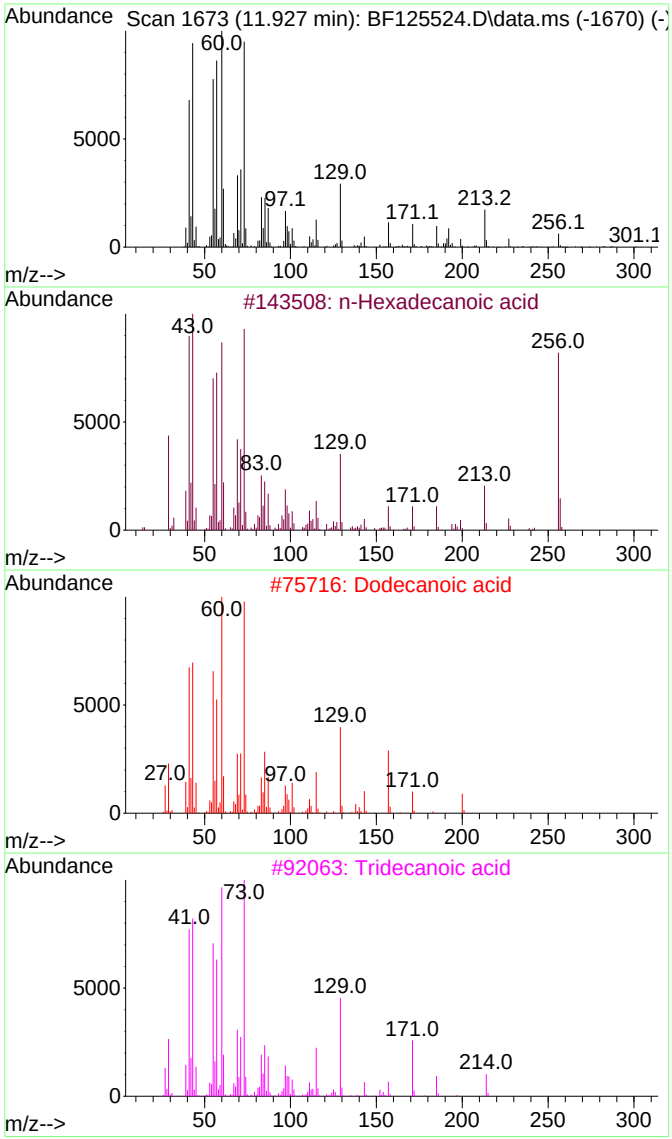
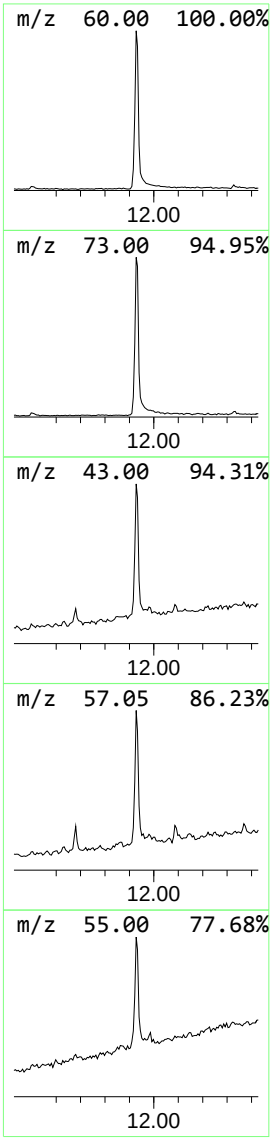
Peak Number 9 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.927	22.22 ng	1117230	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Dodecanoic acid	200	C12H24O2	000143-07-7	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	90
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091521\
Data File : BF125524.D
Acq On : 16 Sep 2021 1:56
Operator : JU/CG
Sample : M3687-21 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A005015

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091521.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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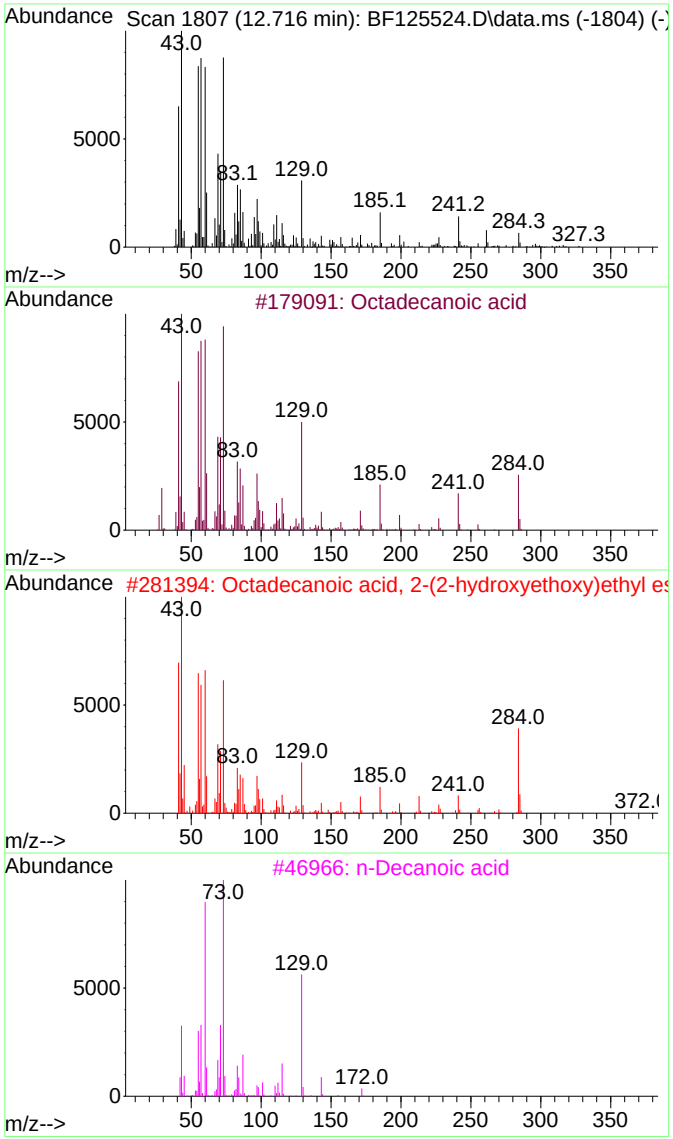
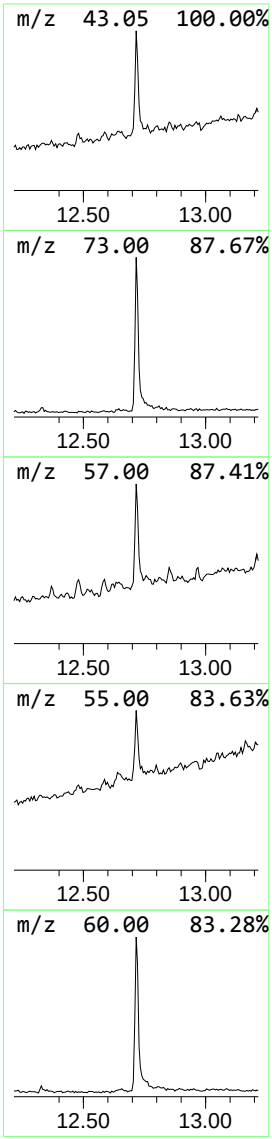
Peak Number 10 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.716	14.66 ng	737334	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
3	n-Decanoic acid	172	C10H20O2	000334-48-5	83
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
5	Dodecanoic acid	200	C12H24O2	000143-07-7	62





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091521\
Data File : BF125524.D
Acq On : 16 Sep 2021 1:56
Operator : JU/CG
Sample : M3687-21 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A005015

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091521.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...	2.134	13.1	ng	629972	1	6.869	964767	20.0
2-Pentanone, 4-...	5.075	6.5	ng	314516	1	6.869	964767	20.0
Hexanoic acid, ...	7.545	2.1	ng	123668	2	8.151	1195410	20.0
Ethanol, 2-(2-b...	8.069	2.6	ng	156974	2	8.151	1195410	20.0
Nonanoic acid	8.551	39.3	ng	2351130	2	8.151	1195410	20.0
n-Decanoic acid	9.104	32.6	ng	1891090	3	9.904	1160870	20.0
Undecanoic acid	9.616	12.0	ng	695303	3	9.904	1160870	20.0
Tetradecane, 1-...	10.804	2.5	ng	126916	4	11.398	1005720	20.0
n-Hexadecanoic ...	11.927	22.2	ng	1117230	4	11.398	1005720	20.0
Octadecanoic acid	12.716	14.7	ng	737334	4	11.398	1005720	20.0