LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090121\
Data File : BF125309.D
Acq On : 1 Sep 2021 16:35
Operator : JU/CG
Sample : M3607-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20211021-SITE-WATER

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: BF125309.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.163	7	13	20	rVB	3143218	4068029	62.45%	9.639%
2	5.522	580	584	587	rBV	2913015	2574695	39.52%	6.100%
3	6.528	751	755	769	rVB	2251332	2006458	30.80%	4.754%
4	6.904	815	819	823	rBV	1367666	1038858	15.95%	2.461%
5	7.469	910	915	918	rBV	3180688	3159607	48.50%	7.486%
6	8.086	1017	1020	1034	rBV	1374009	1558111	23.92%	3.692%
7	8.186	1034	1037	1041	rVB	1665155	1410296	21.65%	3.342%
8	9.269	1216	1221	1224	rBV	5825033	5394582	82.81%	12.782%
9	9.375	1236	1239	1244	rBV	82309	78394	1.20%	0.186%
10	9.945	1327	1336	1340	rBV	2017763	1706562	26.20%	4.043%
11	10.033	1344	1351	1357	rVB5	47361	76914	1.18%	0.182%
12	10.357	1402	1406	1410	rVB3	45912	66067	1.01%	0.157%
13	10.739	1466	1471	1474	rBV	4060078	3854966	59.18%	9.134%
14	10.857	1487	1491	1494	rVB2	71236	69060	1.06%	0.164%
15	11.433	1585	1589	1596	rBV	2128702	1806993	27.74%	4.281%
16	11.816	1650	1654	1658	rVB	1094608	869553	13.35%	2.060%
17	11.951	1672	1677	1681	rBV2	200107	209795	3.22%	0.497%
18	12.292	1732	1735	1741	rVB	218210	170094	2.61%	0.403%
19	12.527	1769	1775	1778	rBV	417125	408104	6.26%	0.967%
20	12.910	1838	1840	1843	rVB	102664	73593	1.13%	0.174%
21	13.021	1854	1859	1863	rBV	6097887	6514245	100.00%	15.435%
22	13.239	1893	1896	1899	rBV	140502	116424	1.79%	0.276%
23	13.480	1931	1937	1945	rBV4	47187	82358	1.26%	0.195%
24	13.586	1949	1955	1957	rBV2	216351	241196	3.70%	0.571%
25	13.915	2007	2011	2013	rBV	248140	233683	3.59%	0.554%
26	13.957	2013	2018	2030	rVB7	38166	130901	2.01%	0.310%
27	14.074	2035	2038	2042	rVB	1680182	1566949	24.05%	3.713%
28	14.227	2061	2064	2068	rBV	275872	242400	3.72%	0.574%
29	14.533	2113	2116	2120	rBV	292334	235826	3.62%	0.559%
30	14.851	2164	2170	2177	rBV2	215836	298072	4.58%	0.706%
31	14.927	2179	2183	2187	rVB	121919	115943	1.78%	0.275%
32	15.198	2225	2229	2234	rBV	150901	170685	2.62%	0.404%
33	15.574	2288	2293	2303	rBV2	1104573	1467798	22.53%	3.478%
34	16.039	2367	2372	2377	rVB2	63596	89672	1.38%	0.212%
35	16.562	2456	2461	2472	rBV2	44968	98227	1.51%	0.233%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090121\
Data File : BF125309.D
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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20211021-SITE-WATER

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

Sum of corrected areas: 42205110

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090121\
Data File : BF125309.D
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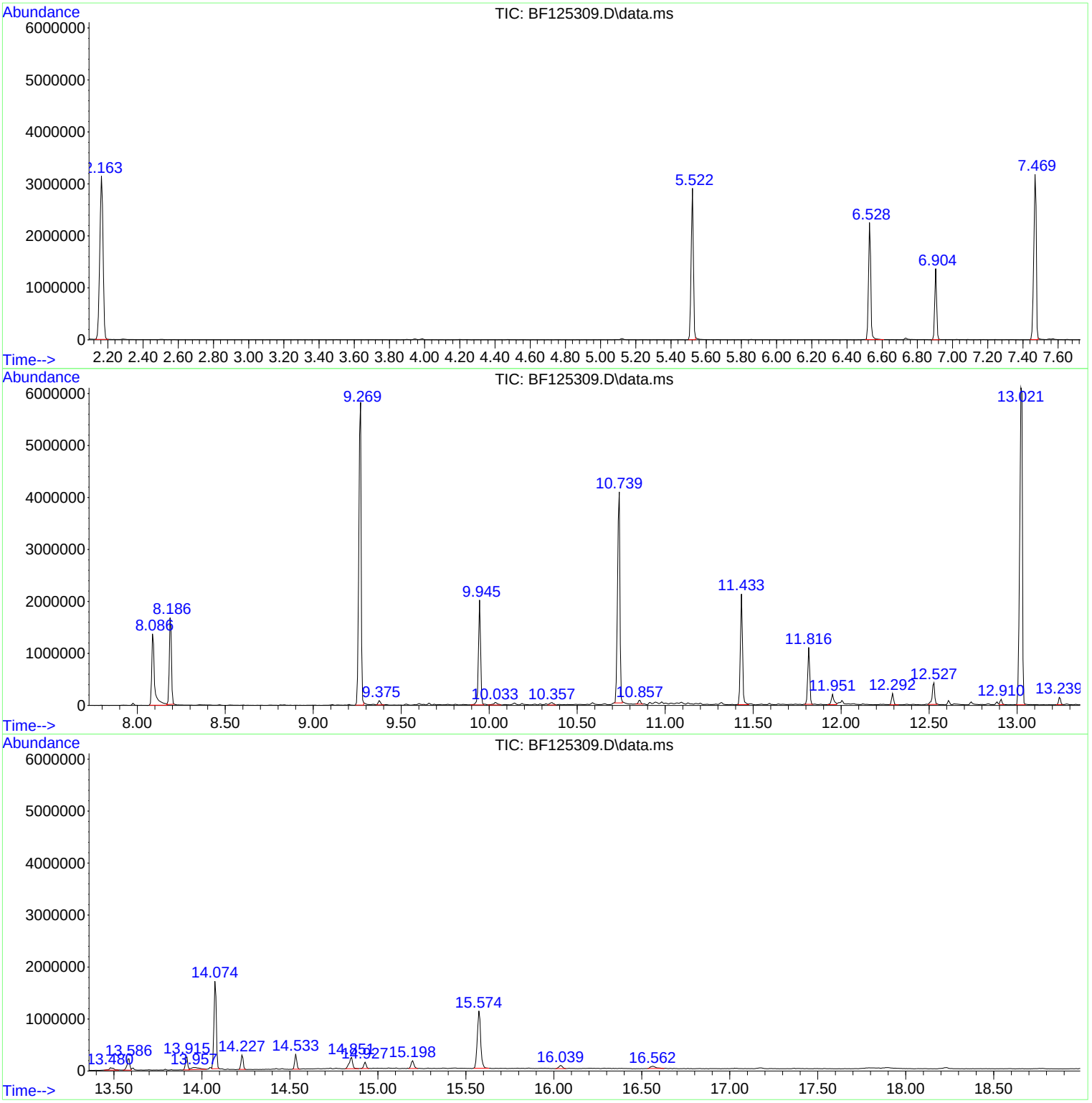
Operator : JU/CG
Sample : M3607-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20211021-SITE-WATER

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\BF090121\
Data File : BF125309.D
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Instrument :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

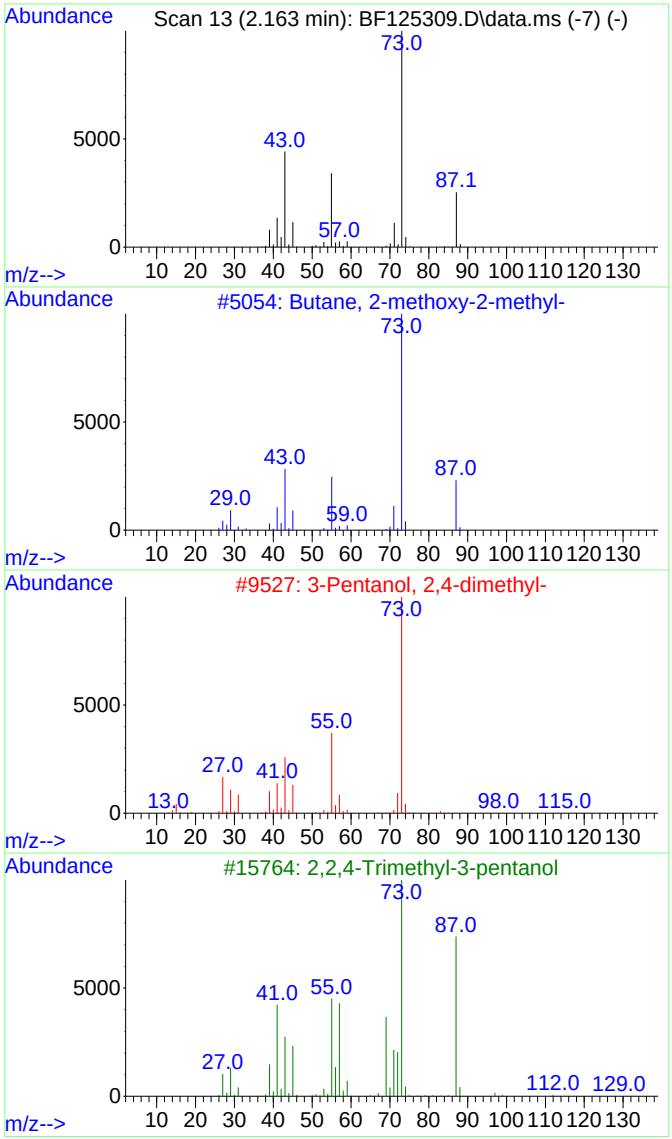
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

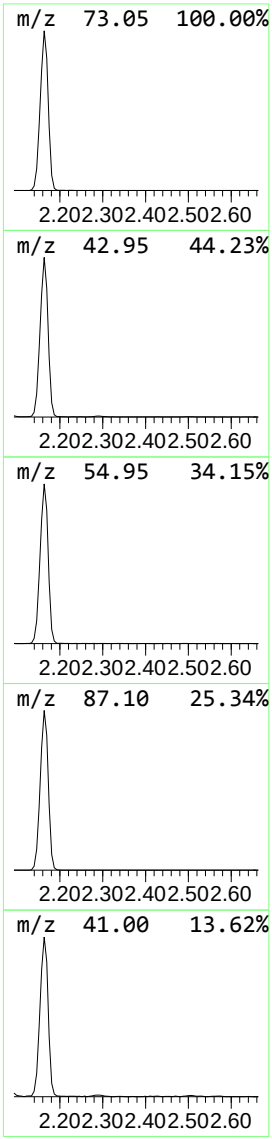
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.163	78.32 ng	4068030	1,4-Dichlorobenzene-d4	6.904

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	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	23





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

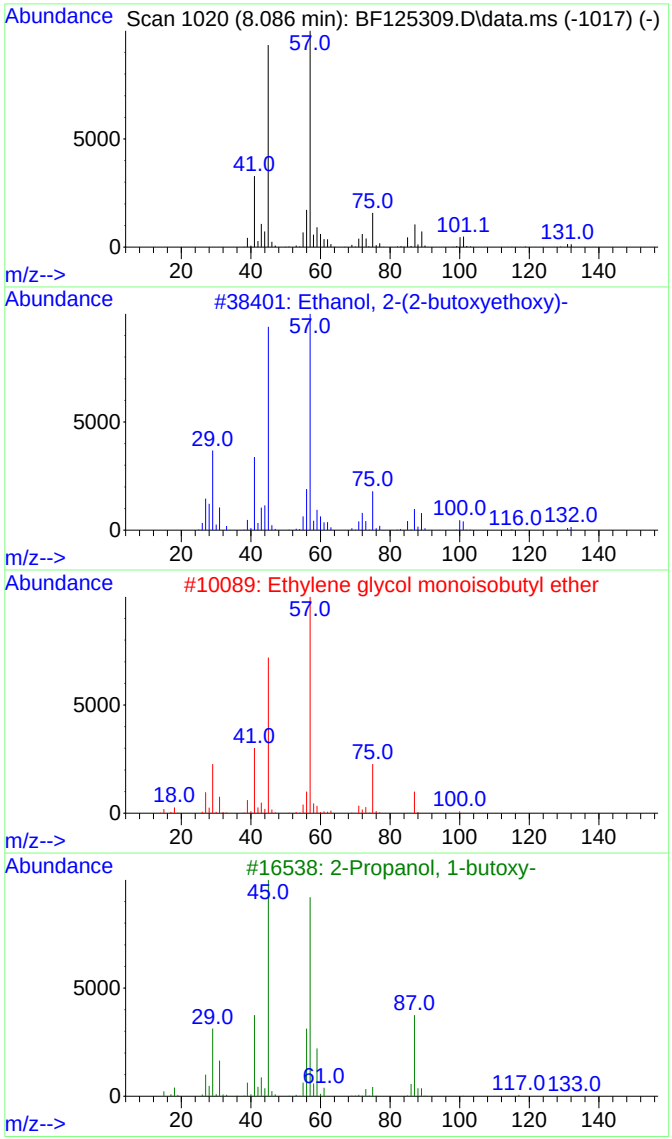
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

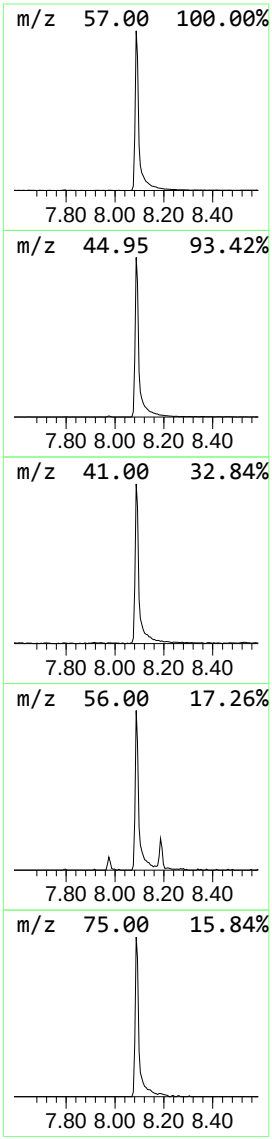
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.086	22.10 ng	1558110	Naphthalene-d8	8.186

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
3	2-Propanol, 1-butoxy-	132	C7H16O2	005131-66-8	59
4	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
5	Methoxyacetic acid, 2-methylprop...	146	C7H14O3	1000282-40-9	53





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Acq On : 1 Sep 2021 16:35
Operator : JU/CG
Sample : M3607-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20211021-SITE-WATER

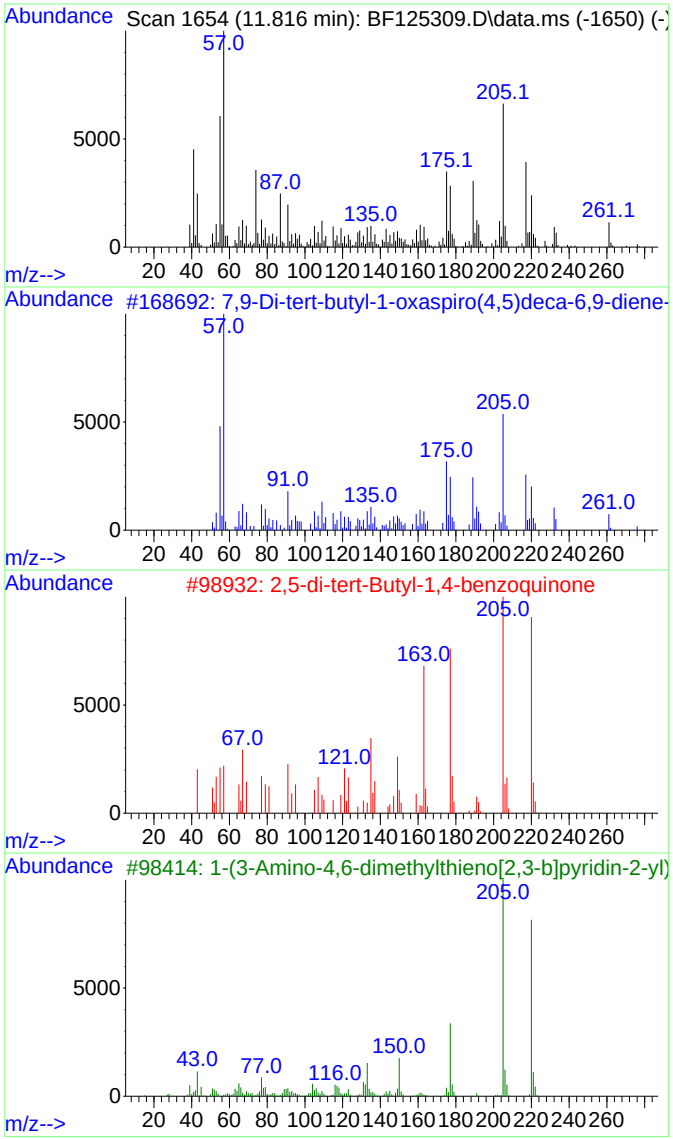
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

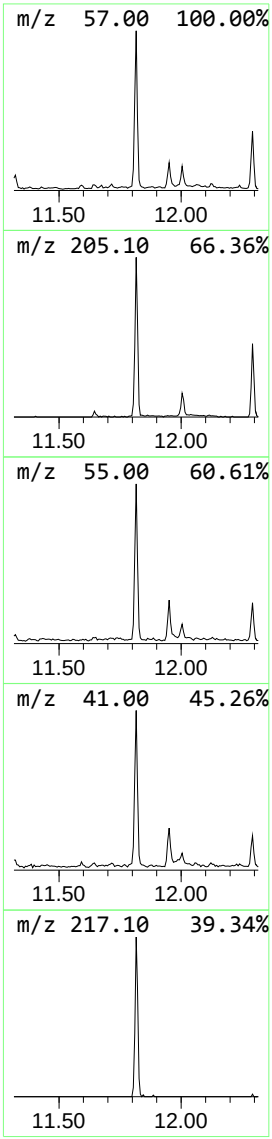
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 7,9-Di-tert-butyl-1-oxaspir... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.816	9.62 ng	869553	Phenanthrene-d10	11.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	97
2	2,5-di-tert-Butyl-1,4-benzoquinone	220	C14H20O2	002460-77-7	60
3	1-(3-Amino-4,6-dimethylthieno[2,...	220	C11H12N2OS	052505-42-7	41
4	Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	41
5	9-Acetylphenanthrene	220	C16H12O	002039-77-2	38





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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
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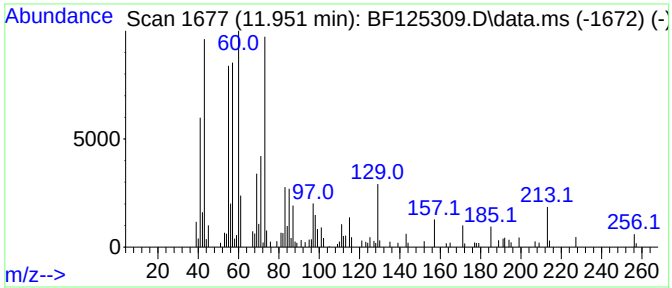
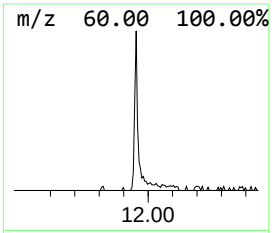
****

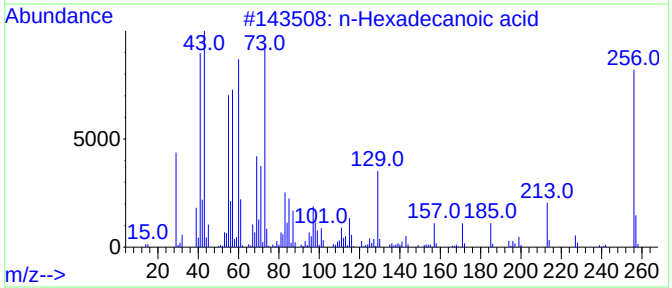
Peak Number 4 n-Hexadecanoic acid Concentration Rank 11

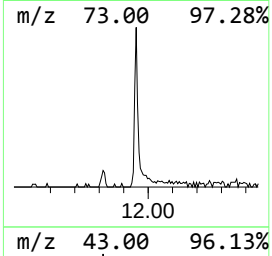
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.951	2.32 ng	209795	Phenanthrene-d10	11.433

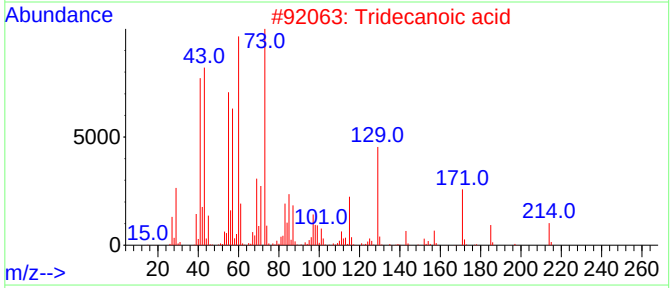
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5	Undecanoic acid	186	C11H22O2	000112-37-8	80

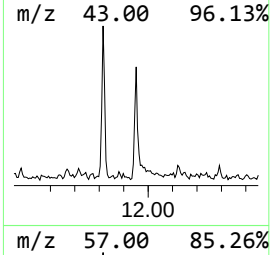


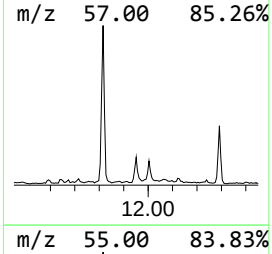


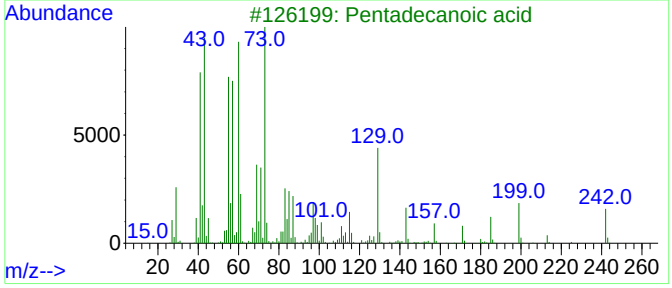


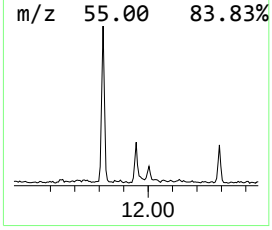












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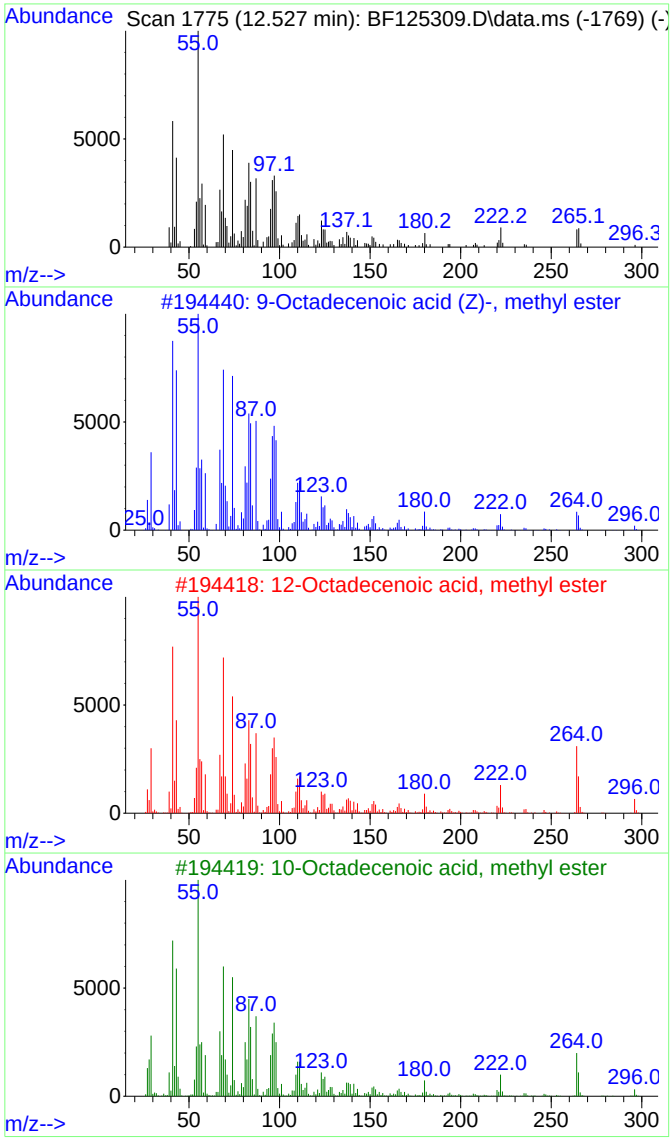
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

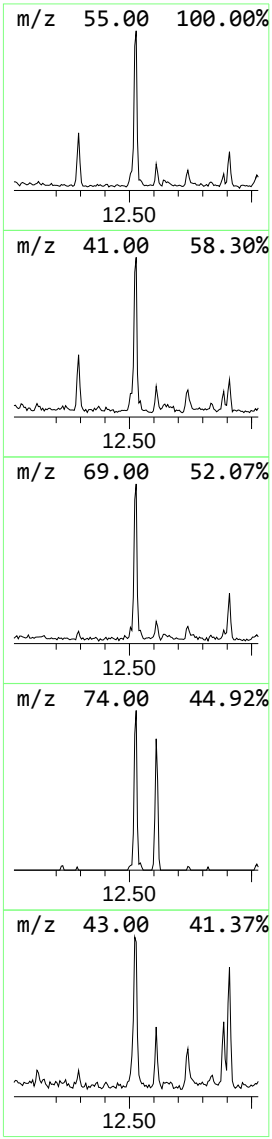
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 9-Octadecenoic acid (Z)-, m... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.527	4.52 ng	408104	Phenanthrene-d10	11.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	99
3	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99
4	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	98
5	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	97





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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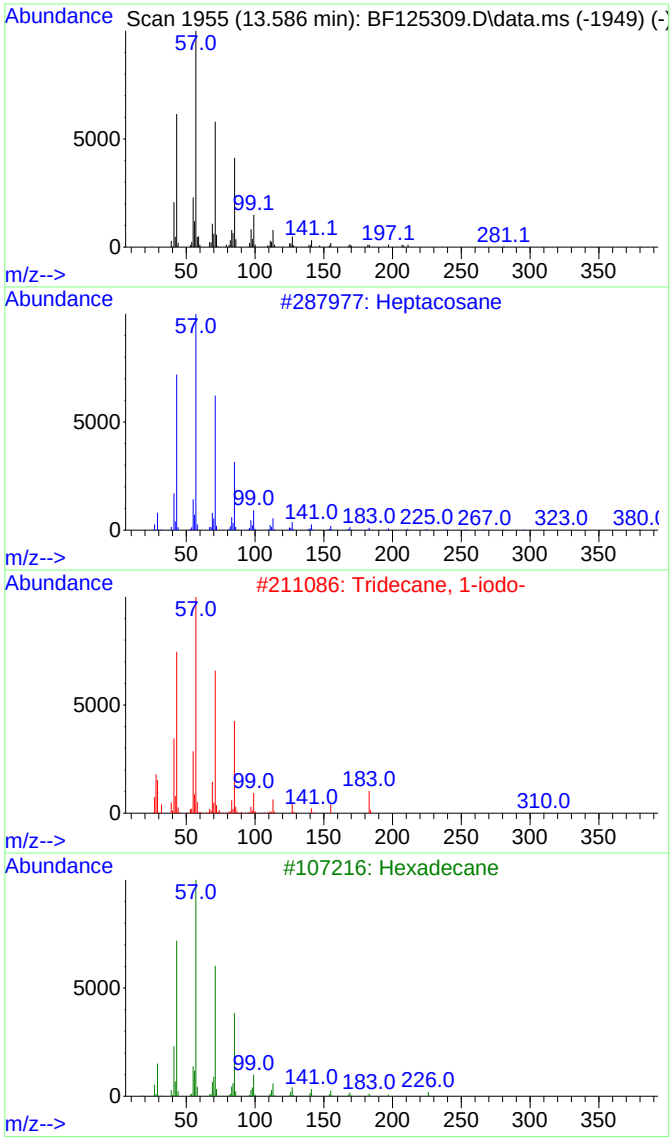
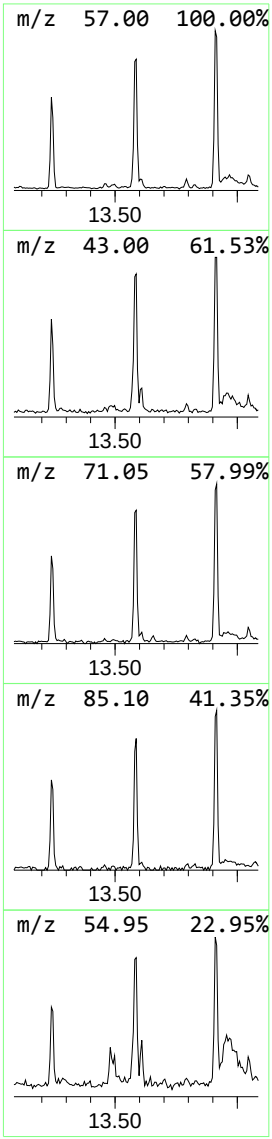
Peak Number 6 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.586	3.08 ng	241196	Chrysene-d12	14.074

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	87
3	Hexadecane	226	C16H34	000544-76-3	87
4	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	86
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86





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Data File : BF125309.D
Acq On : 1 Sep 2021 16:35
Operator : JU/CG
Sample : M3607-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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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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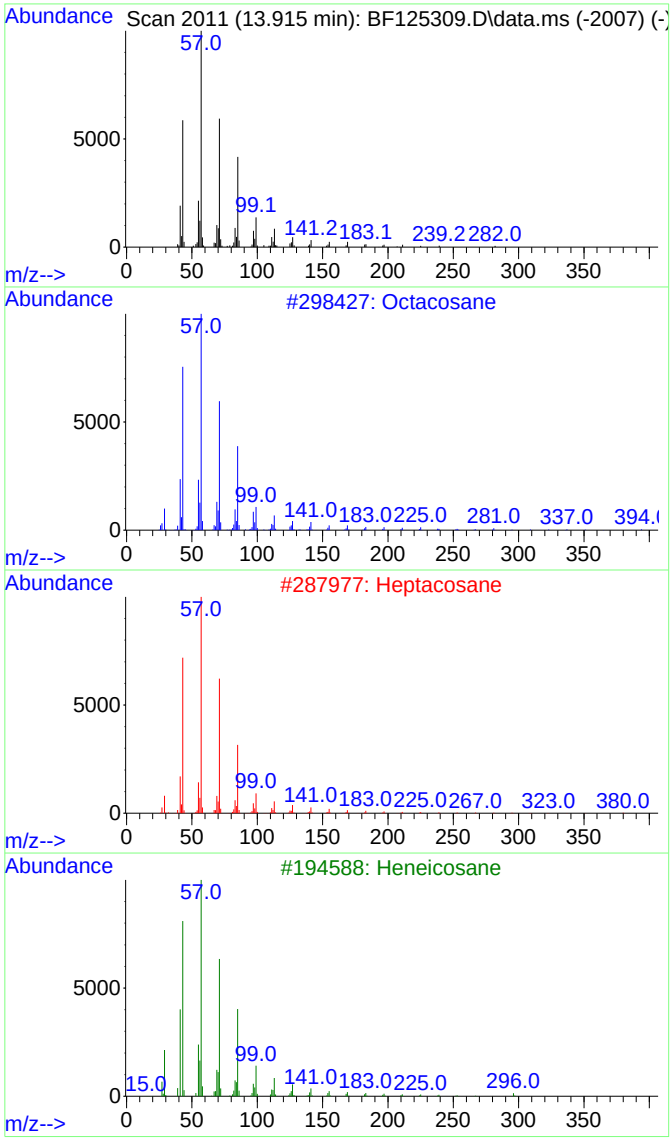
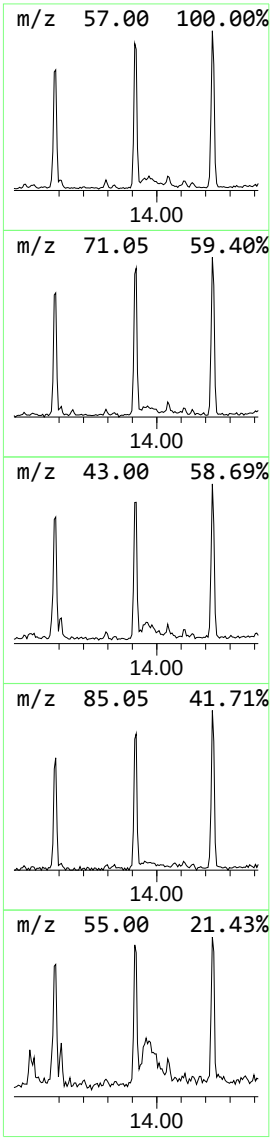
Peak Number 7 Octacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.915	2.98 ng	233683	Chrysene-d12	14.074

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Heptacosane	380	C27H56	000593-49-7	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Docosane	310	C22H46	000629-97-0	91
5	Tetracosane	338	C24H50	000646-31-1	90





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ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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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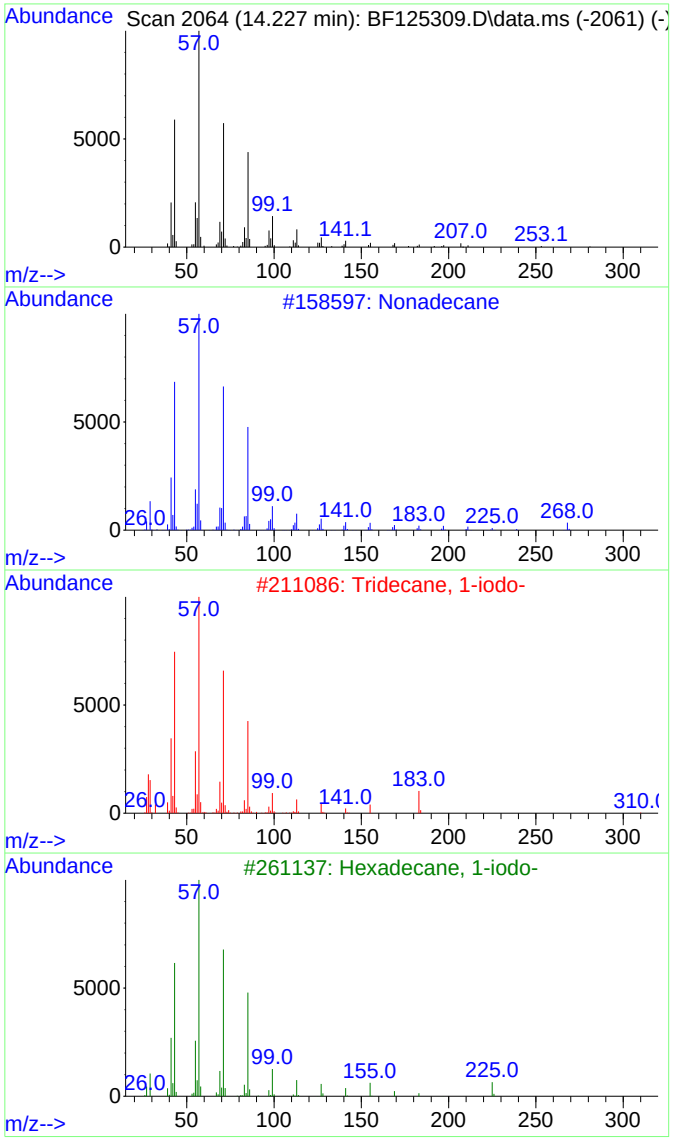
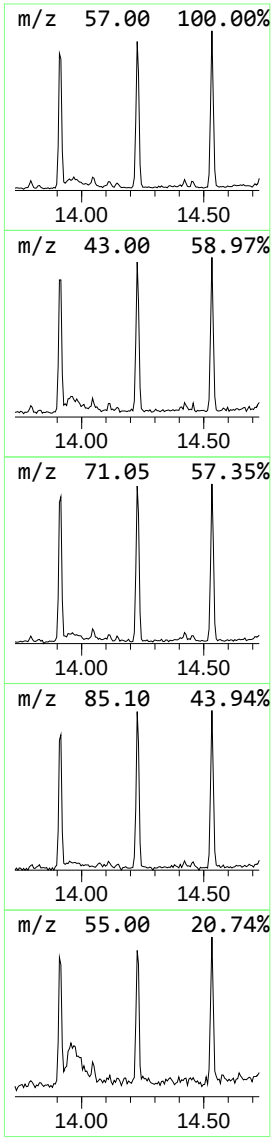
Peak Number 8 Nonadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.227	3.09 ng	242400	Chrysene-d12	14.074

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	90
2	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	87
3	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	86
4	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	86
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090121\
Data File : BF125309.D
Acq On : 1 Sep 2021 16:35
Operator : JU/CG
Sample : M3607-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20211021-SITE-WATER

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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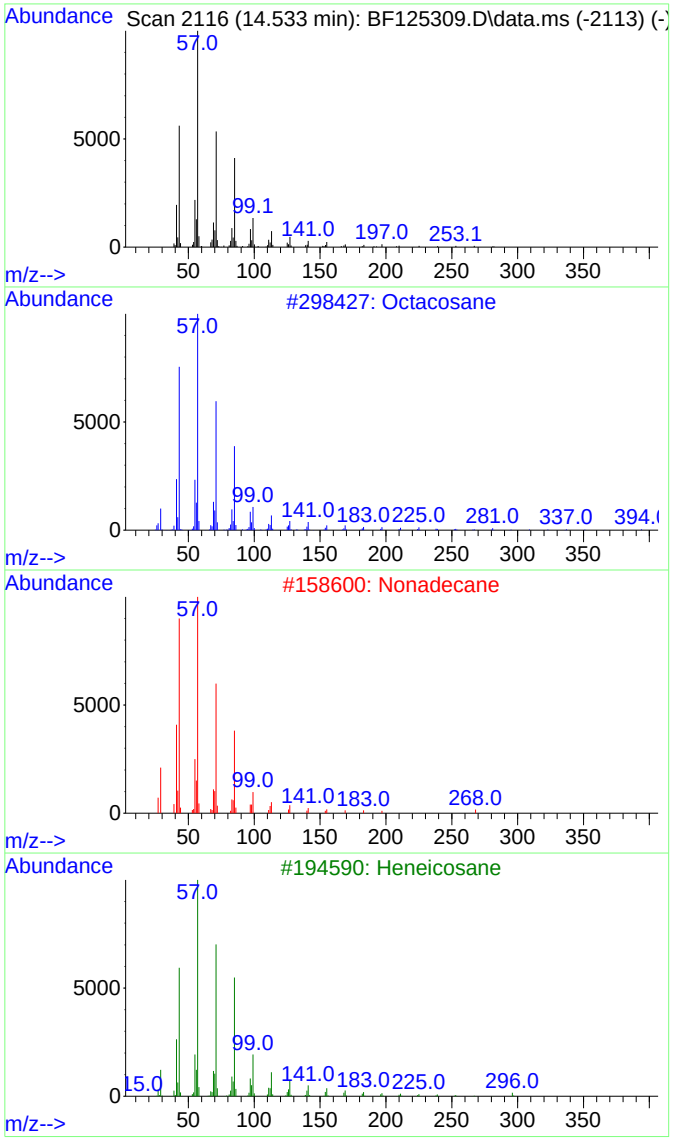
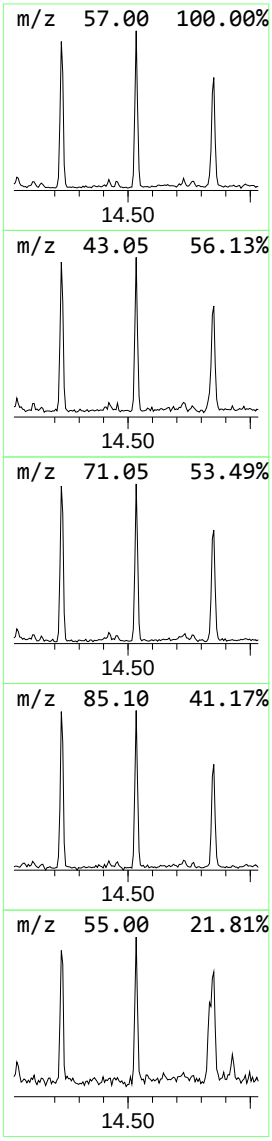
Peak Number 9 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.533	3.01 ng	235826	Chrysene-d12	14.074

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Nonadecane	268	C19H40	000629-92-5	91
3	Heneicosane	296	C21H44	000629-94-7	90
4	Eicosane, 10-methyl-	296	C21H44	054833-23-7	90
5	Heptacosane	380	C27H56	000593-49-7	87





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Data File : BF125309.D
Acq On : 1 Sep 2021 16:35
Operator : JU/CG
Sample : M3607-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20211021-SITE-WATER

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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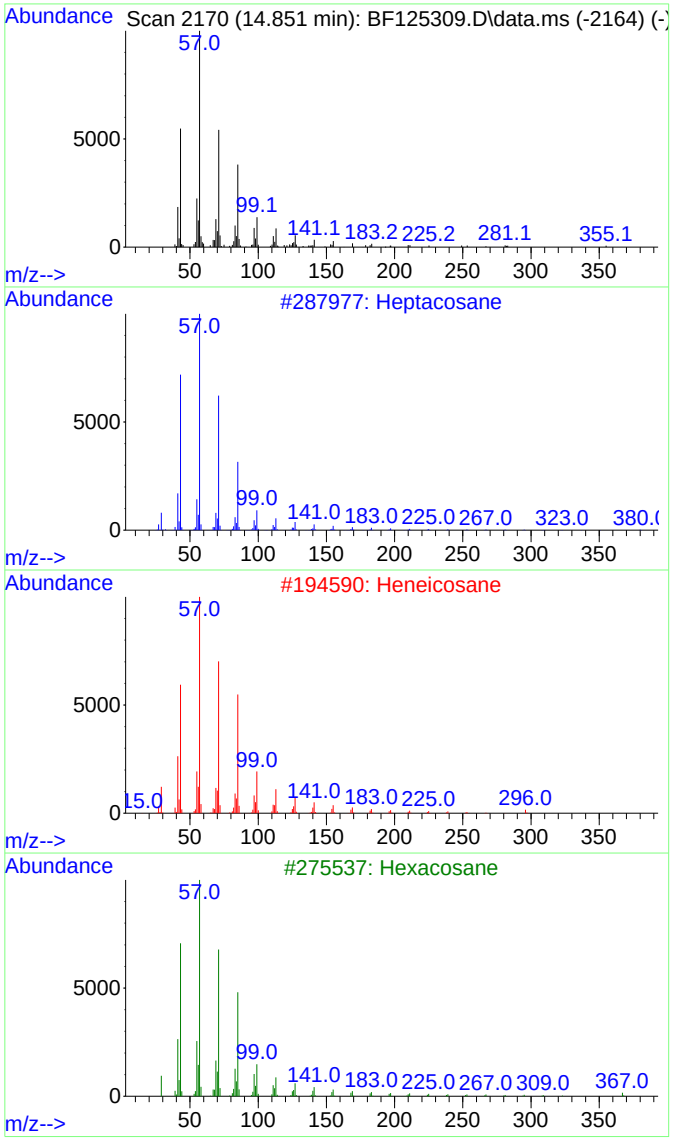
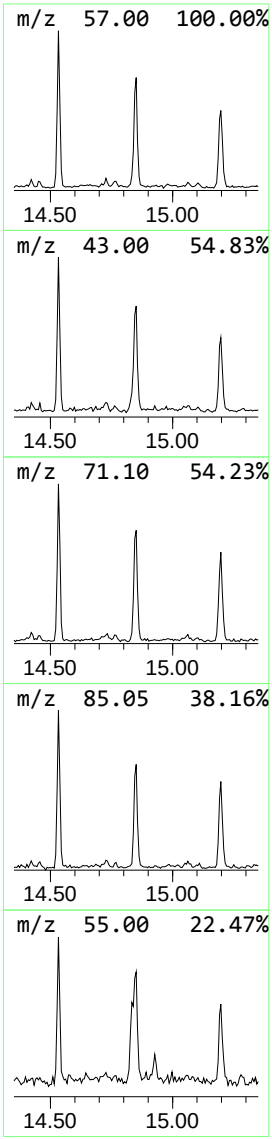
Peak Number 10 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.851	4.06 ng	298072	Perylene-d12	15.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Heneicosane	296	C21H44	000629-94-7	90
3	Hexacosane	366	C26H54	000630-01-3	90
4	Heptadecane	240	C17H36	000629-78-7	87
5	Octadecane	254	C18H38	000593-45-3	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090121\
Data File : BF125309.D
Acq On : 1 Sep 2021 16:35
Operator : JU/CG
Sample : M3607-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20211021-SITE-WATER

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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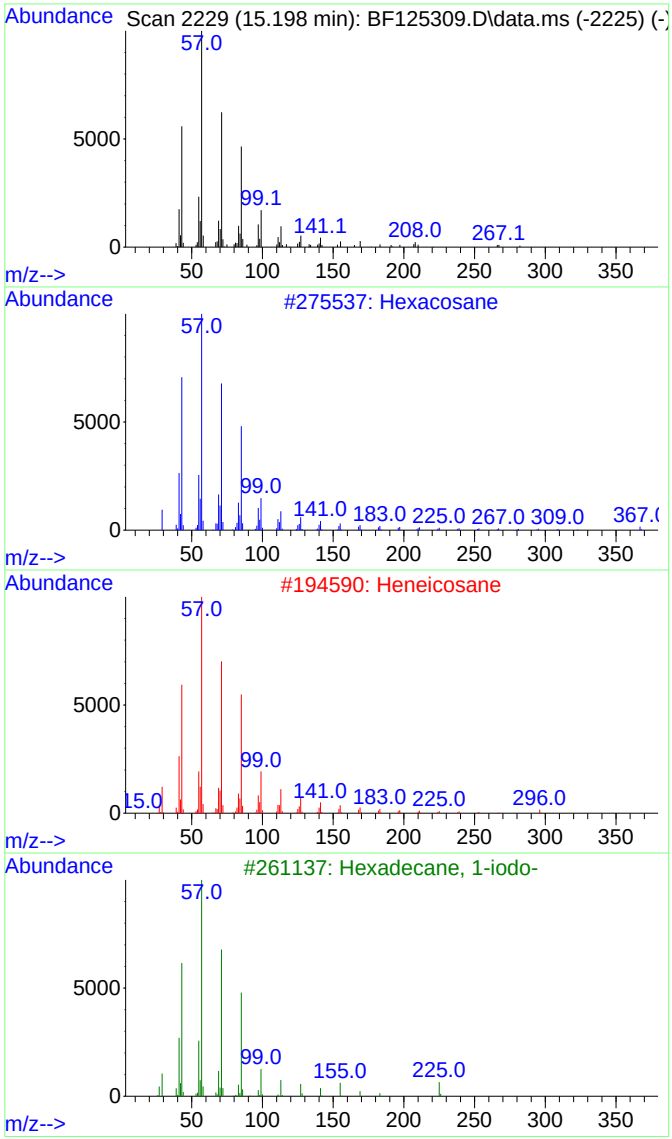
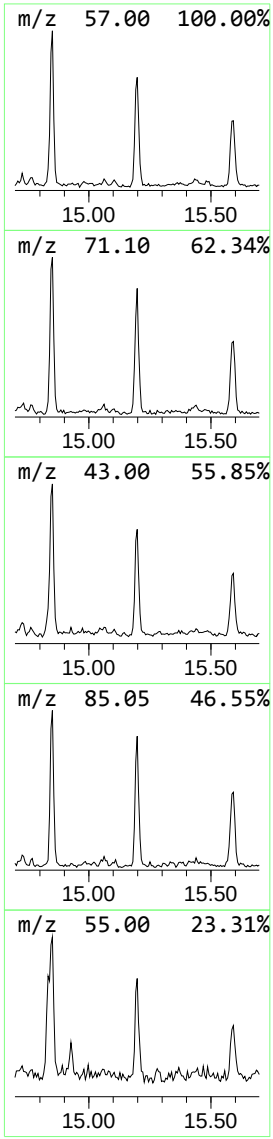
Peak Number 11 Hexadecane, 1-iodo- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.198	2.33 ng	170685	Perylene-d12	15.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Heneicosane	296	C21H44	000629-94-7	90
3	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	87
4	Eicosane	282	C20H42	000112-95-8	87
5	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090121\
Data File : BF125309.D
Acq On : 1 Sep 2021 16:35
Operator : JU/CG
Sample : M3607-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20211021-SITE-WATER

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...	2.163	78.3	ng	4068030	1	6.904	1038860	20.0
Ethanol, 2-(2-b...	8.086	22.1	ng	1558110	2	8.186	1410300	20.0
7,9-Di-tert-but...	11.816	9.6	ng	869553	4	11.433	1806990	20.0
n-Hexadecanoic ...	11.951	2.3	ng	209795	4	11.433	1806990	20.0
9-Octadecenoic ...	12.527	4.5	ng	408104	4	11.433	1806990	20.0
Heptacosane	13.586	3.1	ng	241196	5	14.074	1566950	20.0
Octacosane	13.915	3.0	ng	233683	5	14.074	1566950	20.0
Nonadecane	14.227	3.1	ng	242400	5	14.074	1566950	20.0
Heneicosane	14.533	3.0	ng	235826	5	14.074	1566950	20.0
Hexacosane	14.851	4.1	ng	298072	6	15.574	1467800	20.0
Hexadecane, 1-i...	15.198	2.3	ng	170685	6	15.574	1467800	20.0