LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022520\
Data File : BF119076.D
Acq On : 25 Feb 2020 20:46
Operator : CG/JU
Sample : L1635-18
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIED-TS005-01

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-BF022020.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.987	490	493	504	rVB	40008	58662	1.23%	0.155%
2	5.387	556	561	582	rBV	3403943	3480272	72.87%	9.197%
3	6.398	728	733	747	rBV	3288550	3532288	73.96%	9.334%
4	6.751	789	793	803	rBV	1283561	1104442	23.12%	2.919%
5	6.910	815	820	823	rBV	3279634	3127521	65.48%	8.265%
6	7.316	884	889	892	rBV	2312543	2376099	49.75%	6.279%
7	8.033	1006	1011	1025	rBV	1497966	1486497	31.12%	3.928%
8	9.110	1188	1194	1197	rBV	4846662	4775988	100.00%	12.621%
9	9.498	1257	1260	1265	rBV	227254	218514	4.58%	0.577%
10	9.786	1303	1309	1317	rBV	1862464	1834354	38.41%	4.847%
11	10.575	1438	1443	1456	rBV	3522516	3308038	69.26%	8.742%
12	11.269	1557	1561	1564	rBV	1975148	1839045	38.51%	4.860%
13	11.798	1648	1651	1662	rBV	408262	461591	9.66%	1.220%
14	12.480	1763	1767	1778	rBV	109404	149006	3.12%	0.394%
15	12.580	1780	1784	1794	rBV2	120160	150998	3.16%	0.399%
16	12.704	1802	1805	1807	rBV	72673	63558	1.33%	0.168%
17	12.851	1825	1830	1833	rBV	4927237	4639391	97.14%	12.260%
18	13.080	1864	1869	1872	rBV	75139	76590	1.60%	0.202%
19	13.310	1903	1908	1915	rBV4	51758	98338	2.06%	0.260%
20	13.421	1922	1927	1930	rBV2	120004	121233	2.54%	0.320%
21	13.745	1978	1982	1999	rBV2	512246	770673	16.14%	2.037%
22	13.904	2004	2009	2016	rVV	1418659	1411091	29.55%	3.729%
23	14.068	2032	2037	2045	rBV	179328	200192	4.19%	0.529%
24	14.368	2084	2088	2101	rBV	195399	278930	5.84%	0.737%
25	14.668	2136	2139	2143	rVB	165799	157239	3.29%	0.416%
26	14.739	2147	2151	2154	rBV	119332	112964	2.37%	0.299%
27	14.986	2189	2193	2197	rBV	169214	189527	3.97%	0.501%
28	15.027	2197	2200	2209	rVB	27583	61243	1.28%	0.162%
29	15.327	2246	2251	2268	rVB	930877	1260680	26.40%	3.331%
30	15.751	2319	2323	2328	rBV	114248	165984	3.48%	0.439%
31	15.815	2329	2334	2340	rBV5	36899	87682	1.84%	0.232%
32	16.227	2398	2404	2408	rBV4	50246	97069	2.03%	0.257%
33	17.274	2574	2582	2592	rBV9	46653	146250	3.06%	0.386%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022520\
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Acq On : 25 Feb 2020 20:46
Operator : CG/JU
Sample : L1635-18
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIED-TS005-01

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-BF022020.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

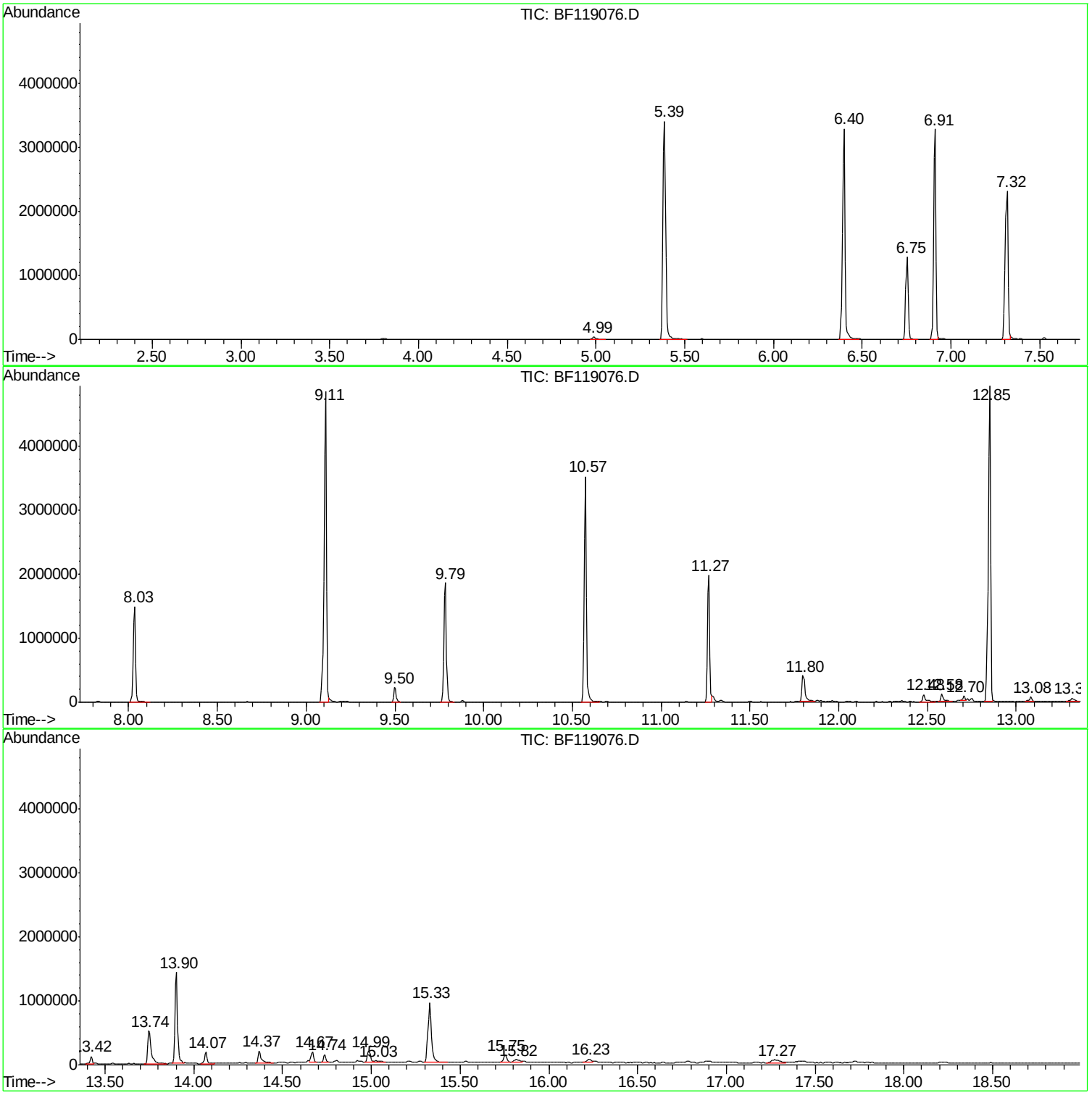
Sum of corrected areas: 37841949

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022520\
Data File : BF119076.D
Acq On : 25 Feb 2020 20:46
Operator : CG/JU
Sample : L1635-18
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LIED-TS005-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022520\
Data File : BF119076.D
Acq On : 25 Feb 2020 20:46
Operator : CG/JU
Sample : L1635-18
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIED-TS005-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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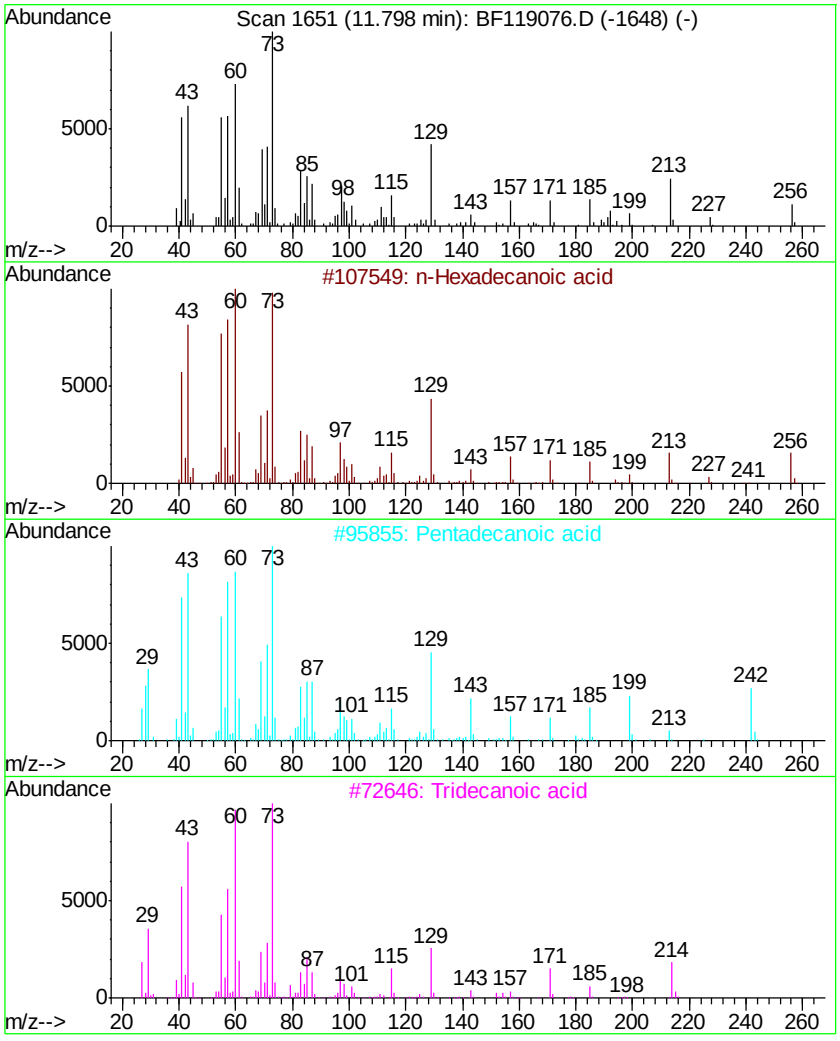
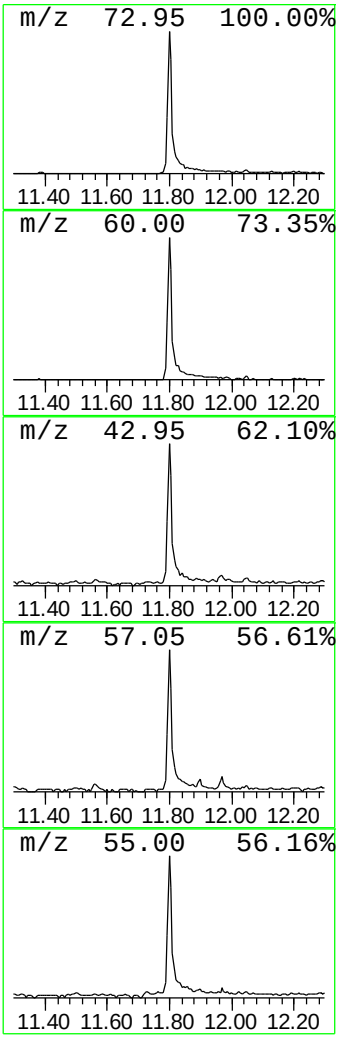
Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.80	5.02 ng	461591	Phenanthrene-d10	11.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	81
4	n-Decanoic acid	172	C10H20O2	000334-48-5	30
5	Oxalic acid, cyclobutyl hexadecy...	368	C22H40O4	1000309-70-6	11





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022520\
Data File : BF119076.D
Acq On : 25 Feb 2020 20:46
Operator : CG/JU
Sample : L1635-18
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIED-TS005-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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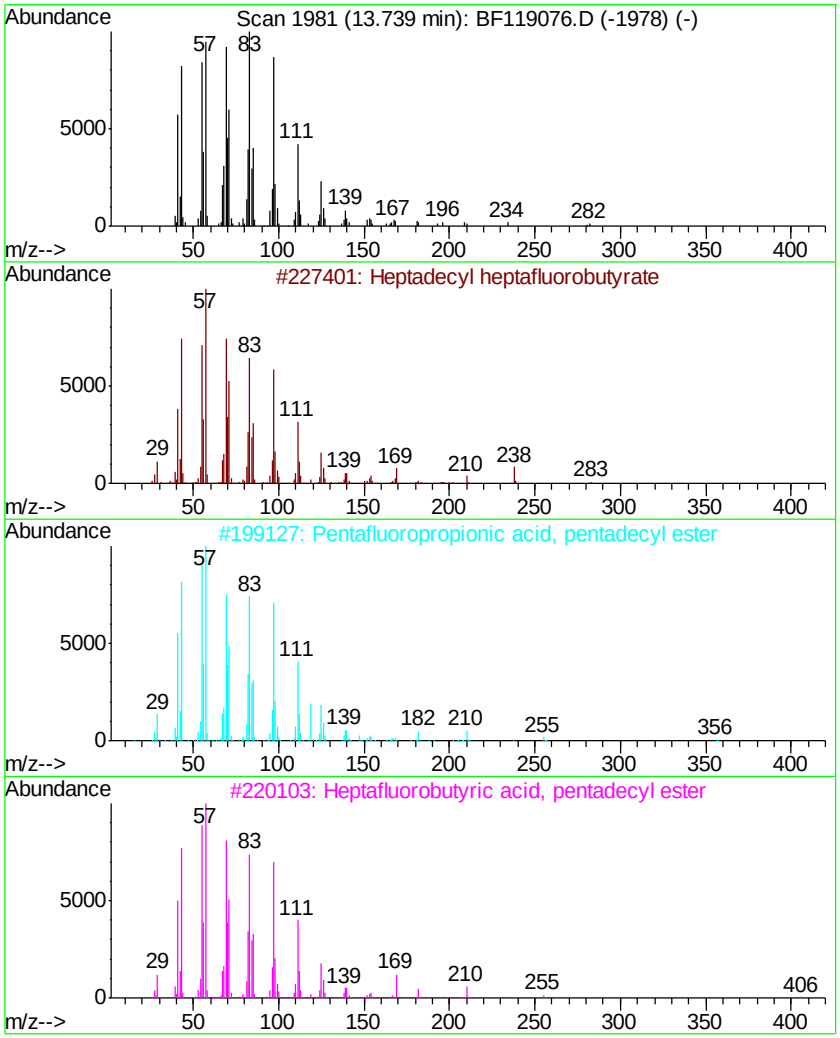
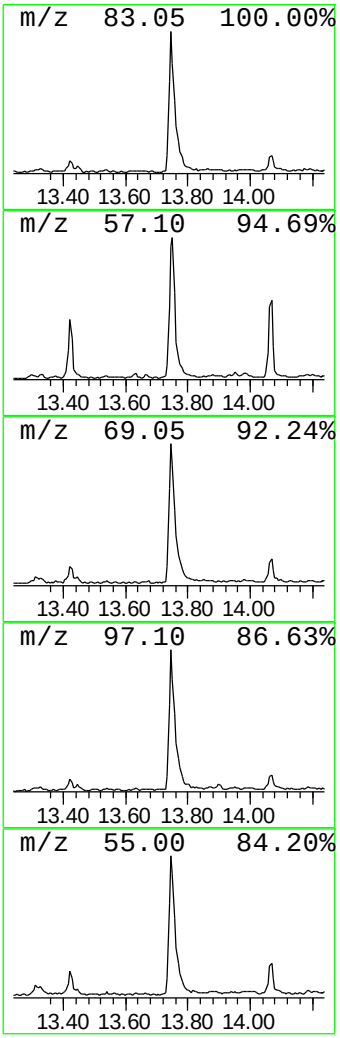
Peak Number 3 Heptadecyl heptafluorobutyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.74	10.92 ng	770673	Chrysene-d12	13.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
4	Behenic alcohol	326	C22H46O	000661-19-8	93
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	93





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022520\
Data File : BF119076.D
Acq On : 25 Feb 2020 20:46
Operator : CG/JU
Sample : L1635-18
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIED-TS005-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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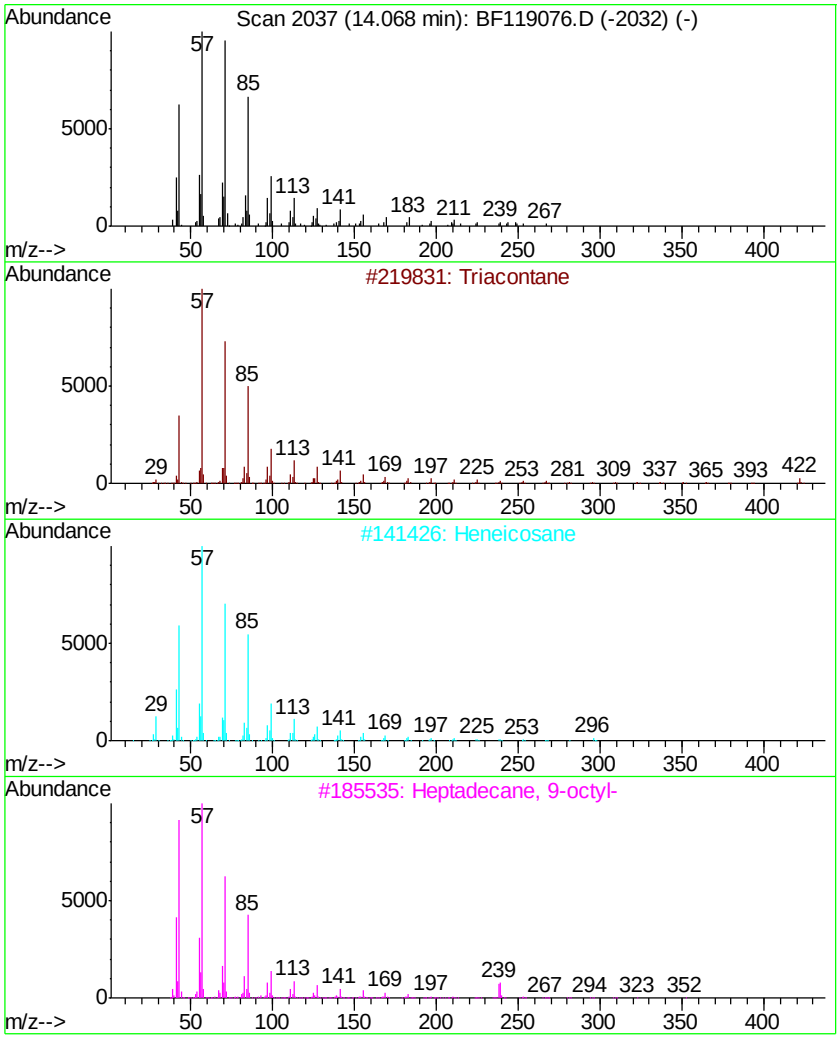
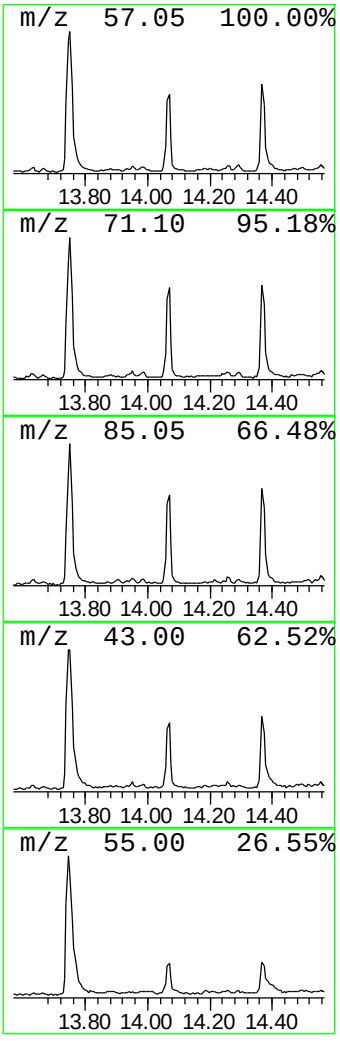
Peak Number 4 Triacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.07	2.84 ng	200192	Chrysene-d12	13.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	91
5	Hexacosane	366	C26H54	000630-01-3	90





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022520\
Data File : BF119076.D
Acq On : 25 Feb 2020 20:46
Operator : CG/JU
Sample : L1635-18
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIED-TS005-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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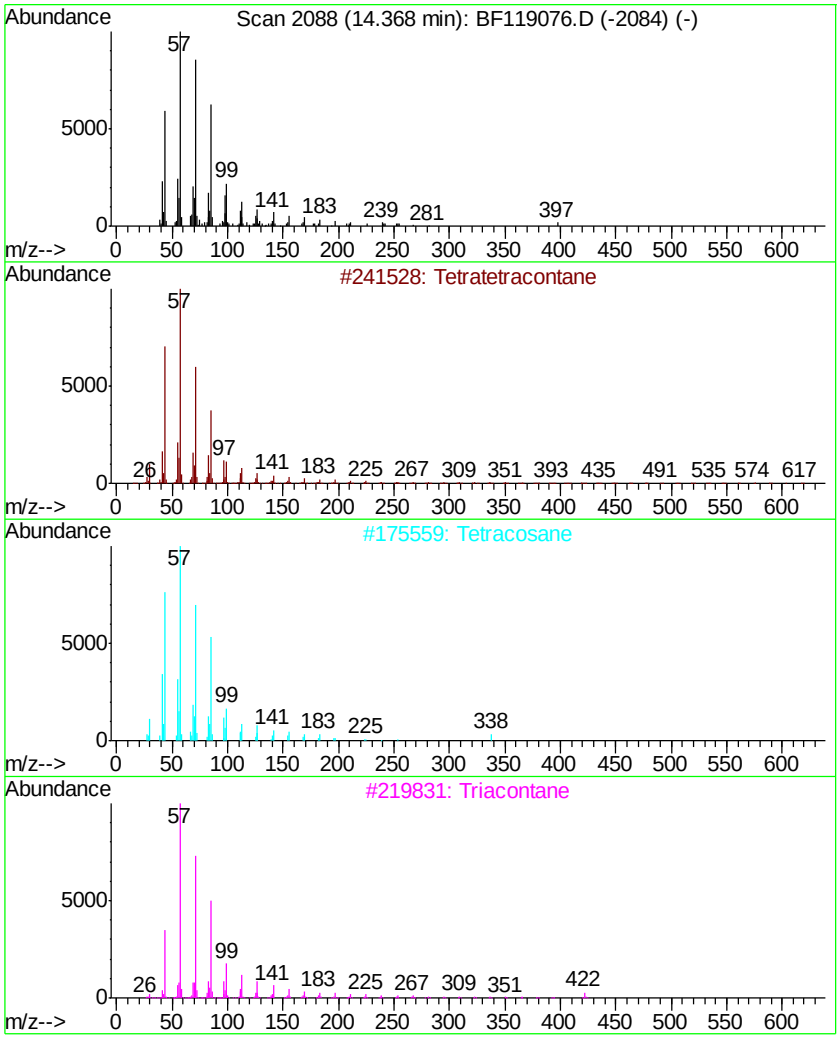
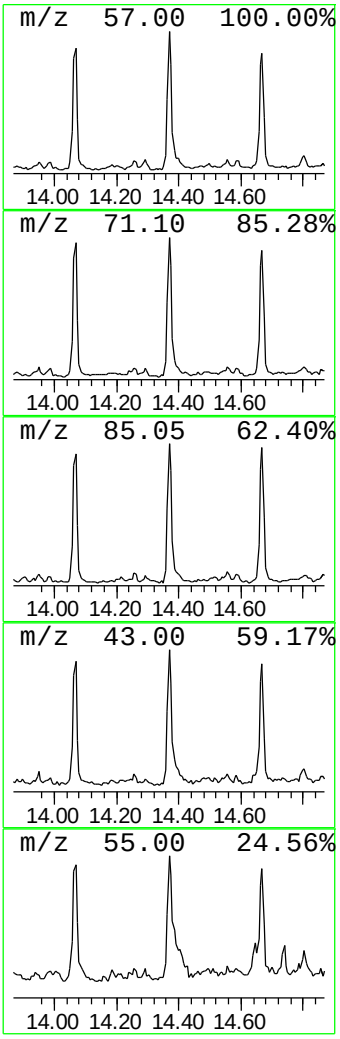
Peak Number 5 Tetratetracontane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.37	3.95 ng	278930	Chrysene-d12	13.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	91
2	Tetracosane	338	C24H50	000646-31-1	91
3	Triacontane	422	C30H62	000638-68-6	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Hexacosane	366	C26H54	000630-01-3	91





Library Search Compound Report

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Operator : CG/JU
Sample : L1635-18
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIED-TS005-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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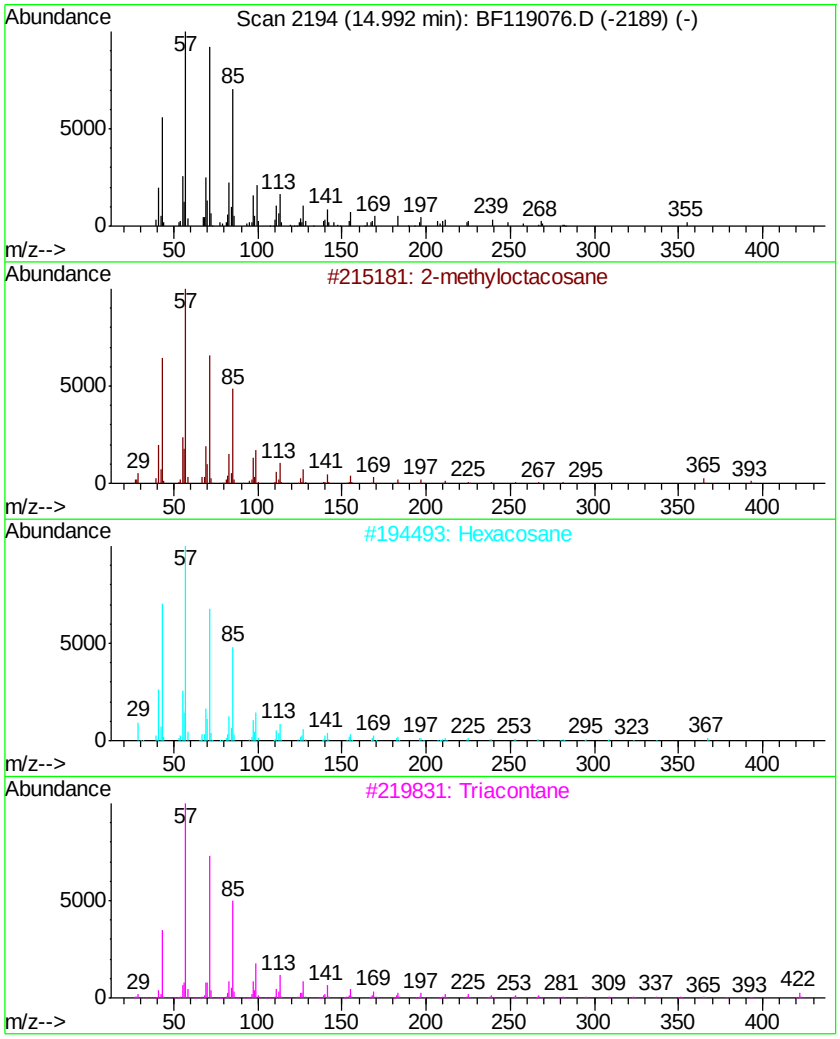
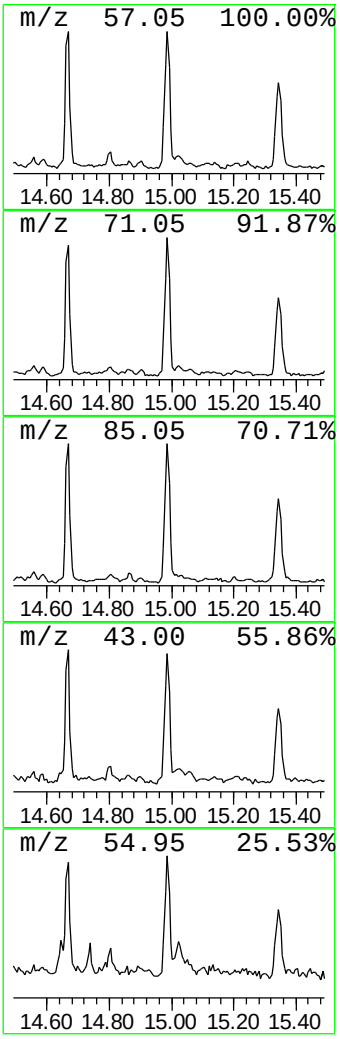
Peak Number 7 2-methyloctacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.99	3.01 ng	189527	Perylene-d12	15.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Triacontane	422	C30H62	000638-68-6	90
4	Hentriacontane	437	C31H64	000630-04-6	87
5	Tetratetracontane	619	C44H90	007098-22-8	87





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Data File : BF119076.D
Acq On : 25 Feb 2020 20:46
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Sample : L1635-18
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIED-TS005-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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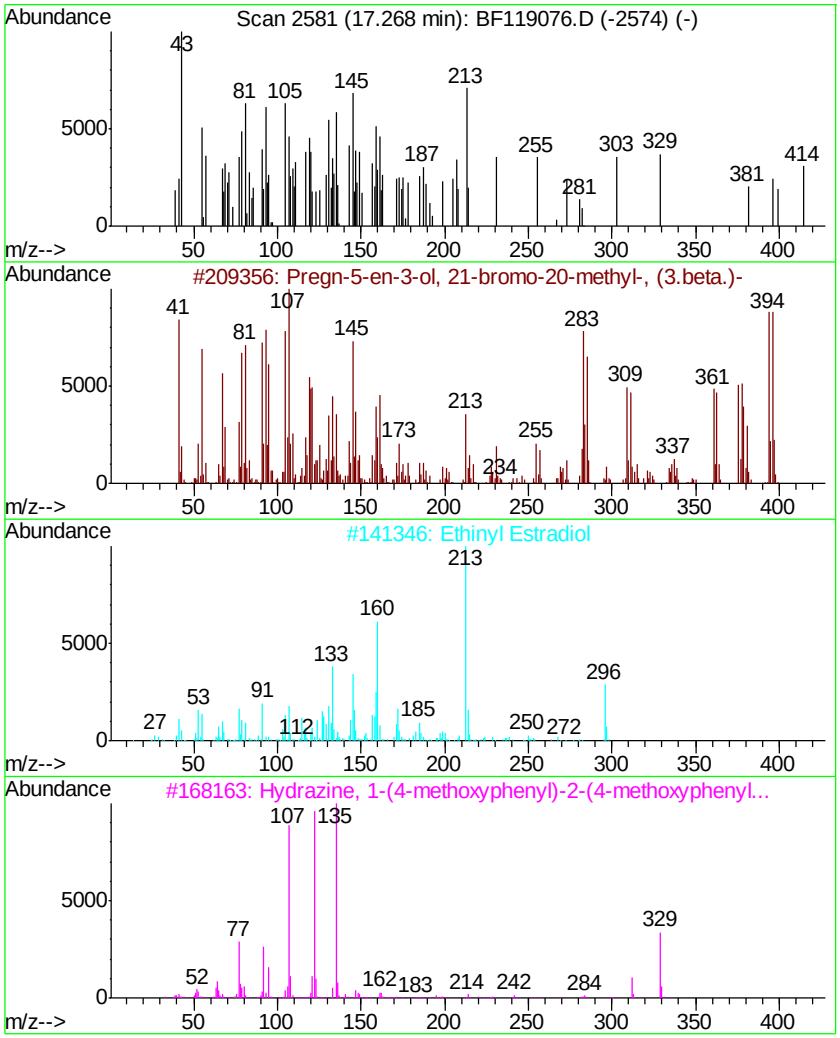
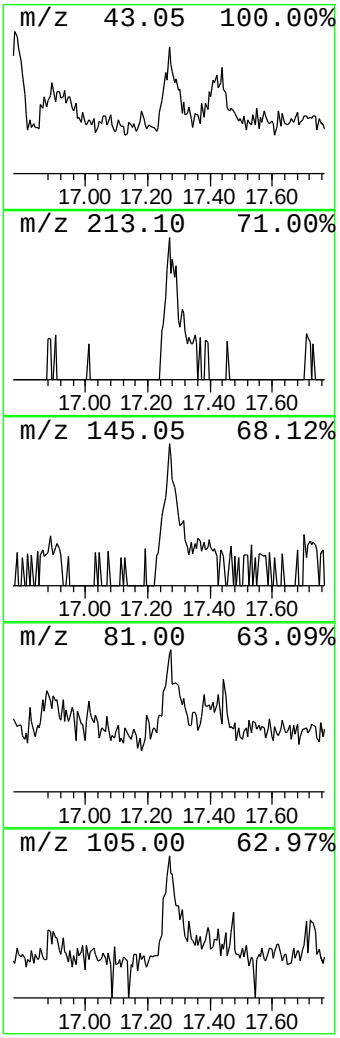
Peak Number 9 unknown17.27 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.27	2.32 ng	146250	Perylene-d12	15.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pregn-5-en-3-ol, 21-bromo-20-met...	394	C22H35BrO	055103-80-5	30
2	Ethinyl Estradiol	296	C20H24O2	000057-63-6	25
3	Hydrazine, 1-(4-methoxyphenyl)-2...	329	C15H15N5O4	051808-28-7	11
4	cis-.alpha.-Copaene-8-ol	220	C15H24O	058569-25-8	10
5	Androst-5-ene,1-acetoxy-16,17-di...	386	C25H38O3	294866-91-4	10





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF022520\
Data File : BF119076.D
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Sample : L1635-18
Misc :
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Instrument : BNA_F
ClientSampleId : LIED-TS005-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
n-Hexadecanoic acid	11.80	5.0	ng	461591	4	11.27	1839050	20.0
Heptadecyl heptaf...	13.74	10.9	ng	770673	5	13.90	1411090	20.0
Triacontane	14.07	2.8	ng	200192	5	13.90	1411090	20.0
Tetratetracontane	14.37	4.0	ng	278930	5	13.90	1411090	20.0
2-methyloctacosane	14.99	3.0	ng	189527	6	15.33	1260680	20.0
unknown17.27	17.27	2.3	ng	146250	6	15.33	1260680	20.0