LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031120\
Data File : BF119349.D
Acq On : 11 Mar 2020 16:21
Operator : CG/JU
Sample : L1864-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1

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	4.904	476	479	492	rBV	171887	253803	8.19%	0.728%
2	5.351	552	555	575	rBV	711727	1645667	53.08%	4.718%
3	5.510	579	582	603	rVB	141561	382788	12.35%	1.097%
4	6.375	725	729	742	rBV	1919388	2209942	71.28%	6.336%
5	6.716	783	787	798	rBV	642025	604364	19.49%	1.733%
6	6.869	809	813	831	rVB	2085611	1963034	63.31%	5.628%
7	7.281	879	883	896	rBV	1458138	1507975	48.64%	4.323%
8	7.998	1001	1005	1021	rBV	843625	796546	25.69%	2.284%
9	9.069	1183	1187	1191	rBV	3066544	2921501	94.22%	8.376%
10	9.469	1251	1255	1263	rVB	427887	367070	11.84%	1.052%
11	9.751	1299	1303	1307	rBV	1007176	961175	31.00%	2.756%
12	10.545	1434	1438	1447	rBV	2003378	2028903	65.44%	5.817%
13	10.916	1496	1501	1509	rBV7	17704	35063	1.13%	0.101%
14	11.233	1552	1555	1559	rBV	1142886	1000314	32.26%	2.868%
15	11.763	1638	1645	1658	rBV	339987	519644	16.76%	1.490%
16	11.928	1669	1673	1677	rBV2	45149	66136	2.13%	0.190%
17	12.457	1759	1763	1771	rBV	61558	93338	3.01%	0.268%
18	12.545	1771	1778	1790	rBV	226394	325263	10.49%	0.933%
19	12.686	1799	1802	1804	rBV	54421	51879	1.67%	0.149%
20	12.816	1820	1824	1827	rBV	3574755	3100584	100.00%	8.889%
21	13.039	1856	1862	1866	rBV2	42062	59440	1.92%	0.170%
22	13.274	1895	1902	1909	rBV9	34045	91390	2.95%	0.262%
23	13.380	1915	1920	1928	rVB2	77009	107611	3.47%	0.309%
24	13.651	1959	1966	1969	rBV5	34059	76832	2.48%	0.220%
25	13.710	1969	1976	1990	rVB2	331817	574248	18.52%	1.646%
26	13.874	2001	2004	2013	rBV	761564	869726	28.05%	2.493%
27	14.021	2025	2029	2036	rVB	442455	526232	16.97%	1.509%
28	14.327	2076	2081	2085	rBV	967845	1157459	37.33%	3.318%
29	14.627	2126	2132	2136	rBV	1690600	1924593	62.07%	5.518%
30	14.692	2141	2143	2147	rVB	42521	40406	1.30%	0.116%
31	14.939	2177	2185	2190	rBV	1829950	2403348	77.51%	6.890%
32	15.157	2218	2222	2224	rBV	42858	52635	1.70%	0.151%
33	15.298	2237	2246	2259	rVB2	1834240	3071114	99.05%	8.805%
34	15.533	2282	2286	2290	rVB2	46908	63096	2.03%	0.181%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031120\
Data File : BF119349.D
Acq On : 11 Mar 2020 16:21
Operator : CG/JU
Sample : L1864-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1

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

35	15.692	2306	2313	2321	rBV	1104193	1755532	56.62%	5.033%
36	16.157	2383	2392	2406	rVB	500232	952895	30.73%	2.732%
37	16.692	2477	2483	2493	rVB2	120366	252460	8.14%	0.724%
38	17.333	2588	2592	2598	rVB3	31768	66498	2.14%	0.191%

Sum of corrected areas: 34880504

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031120\
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Instrument :
BNA_F
ClientSampleId :
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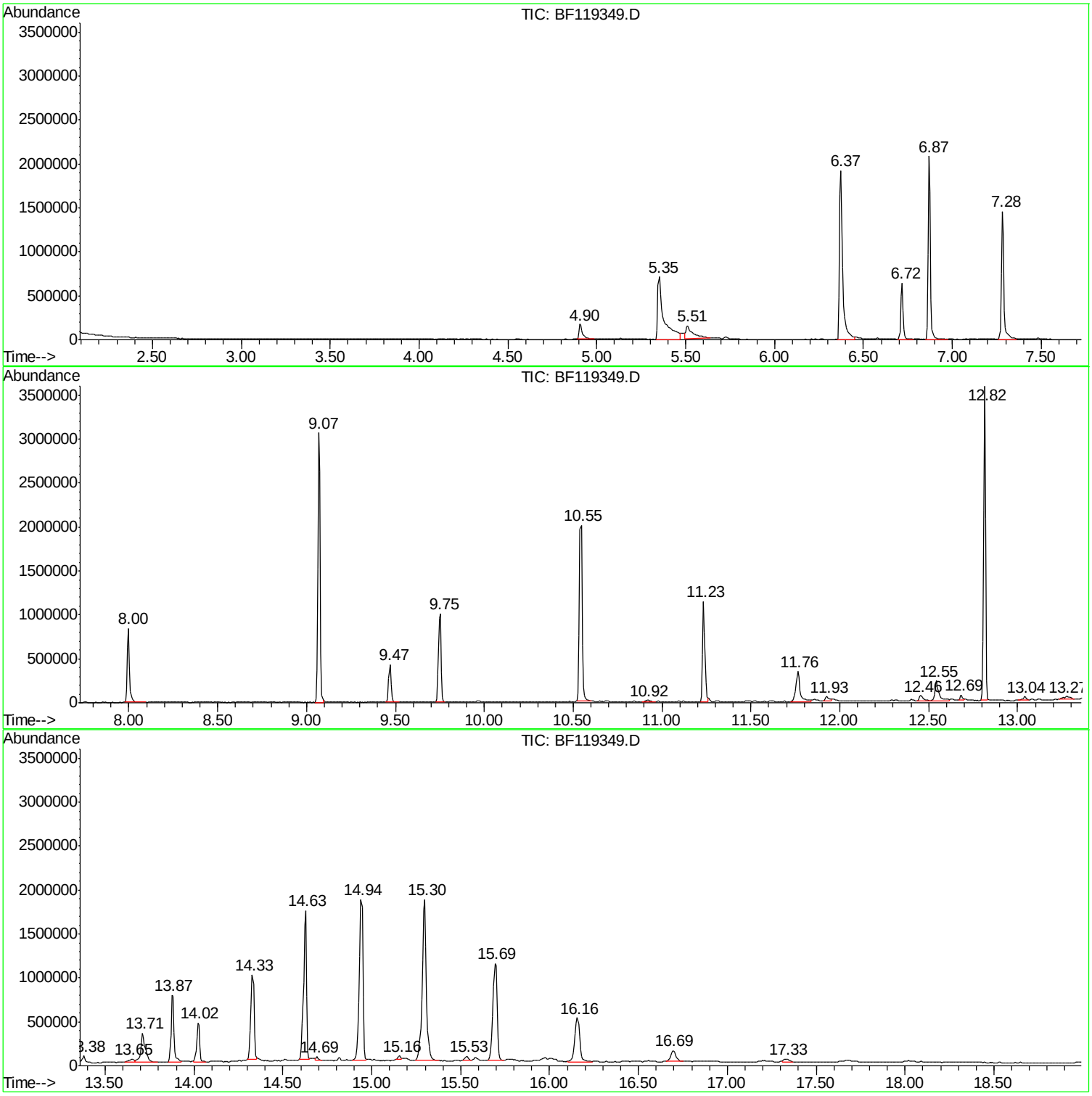
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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Data File : BF119349.D
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Operator : CG/JU
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BNA_F
ClientSampleId :
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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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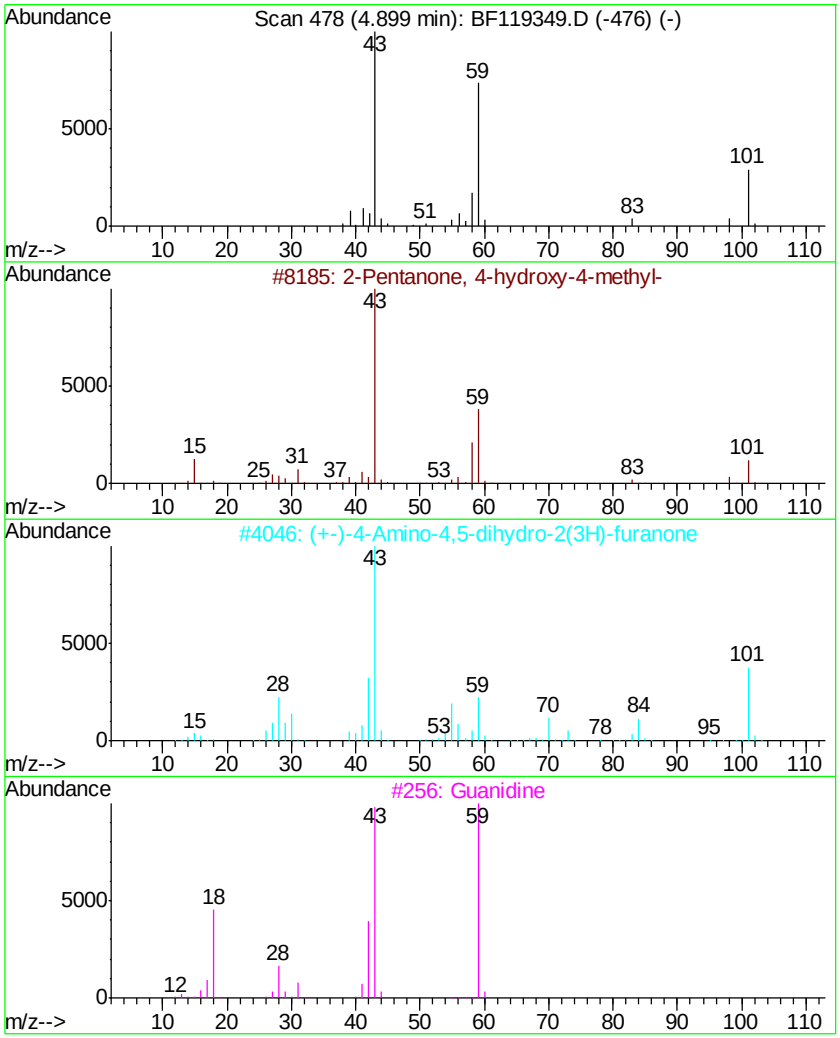
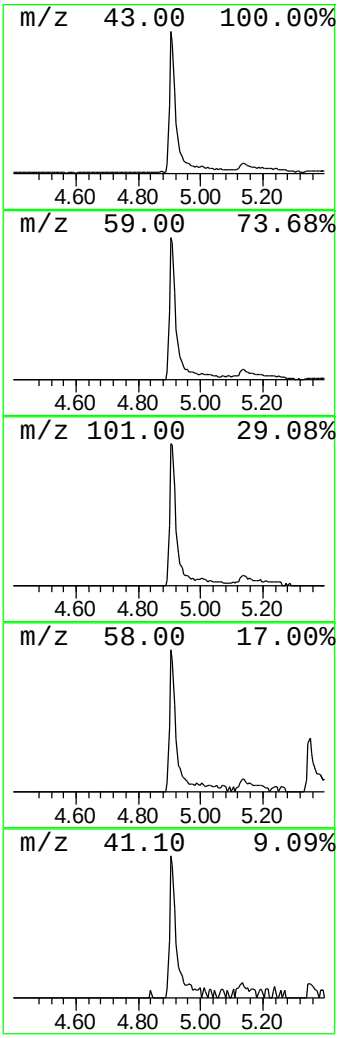
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	8.40 ng	253803	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	47
3	Guanidine	59	CH5N3	000113-00-8	43
4	2,3-Dimethyloxirane-2-carboxylic...	130	C6H10O3	1000306-64-4	28
5	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	25





Library Search Compound Report

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Misc :
ALS Vial : 3 Sample Multiplier: 1

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

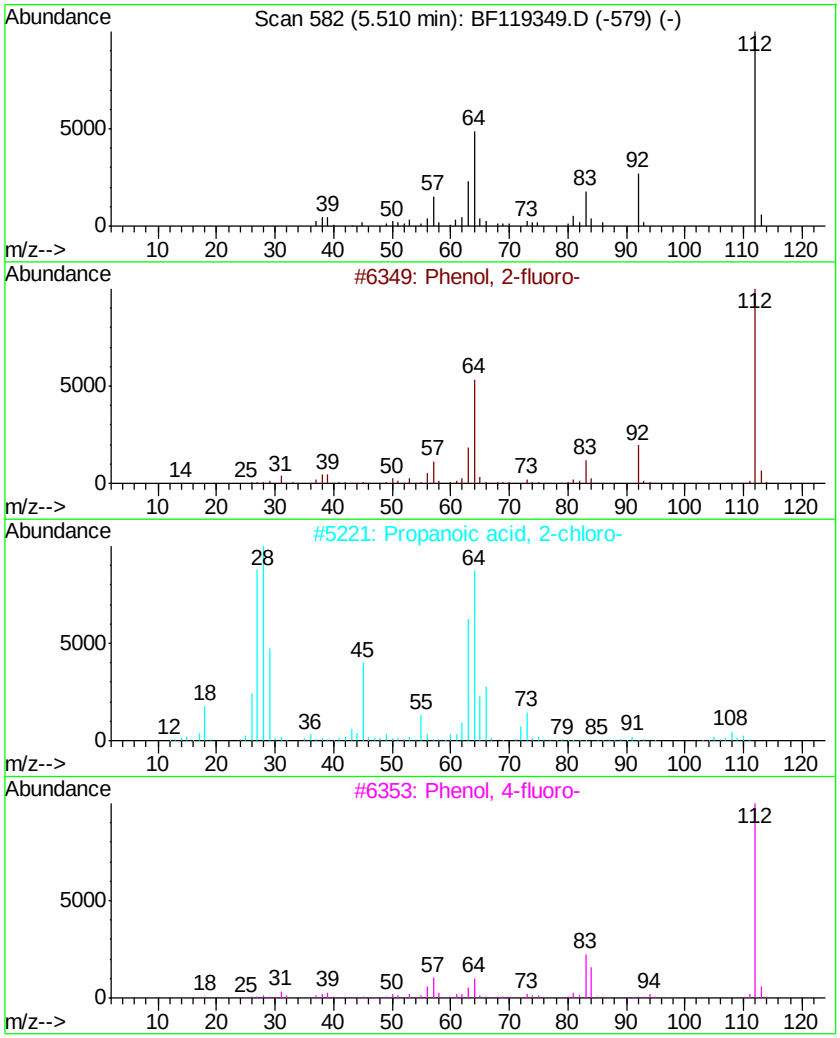
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

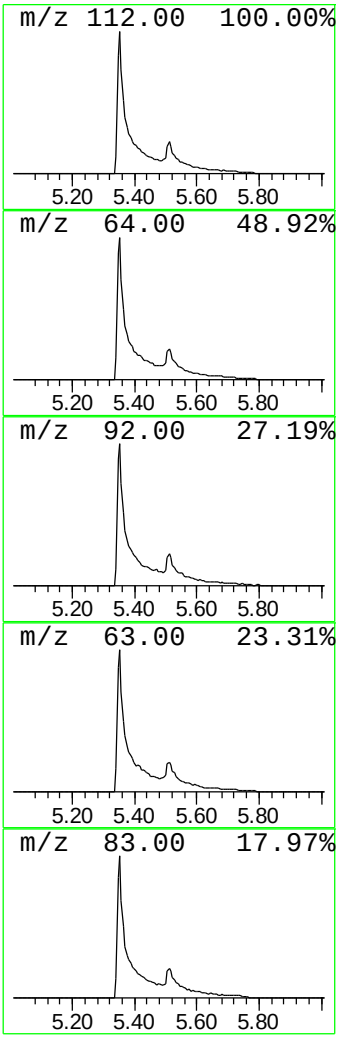
****

Peak Number 2 Phenol, 2-fluoro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.51	12.67 ng	382788	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2-fluoro-	112	C6H5FO	000367-12-4	91
2	Propanoic acid, 2-chloro-	108	C3H5ClO2	000598-78-7	28
3	Phenol, 4-fluoro-	112	C6H5FO	000371-41-5	22
4	1,4-Cyclohexanedione	112	C6H8O2	000637-88-7	10
5	5-Imidazolic acid	112	C4H4N2O2	1000116-93-3	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031120\
Data File : BF119349.D
Acq On : 11 Mar 2020 16:21
Operator : CG/JU
Sample : L1864-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1

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

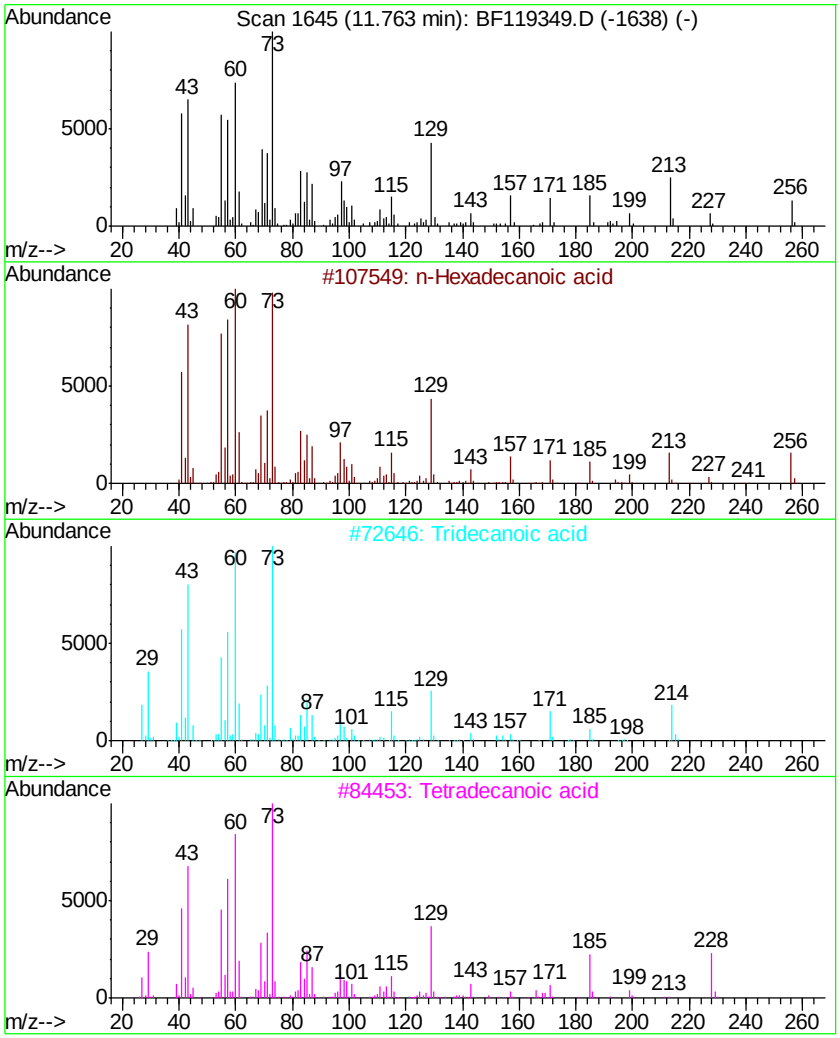
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

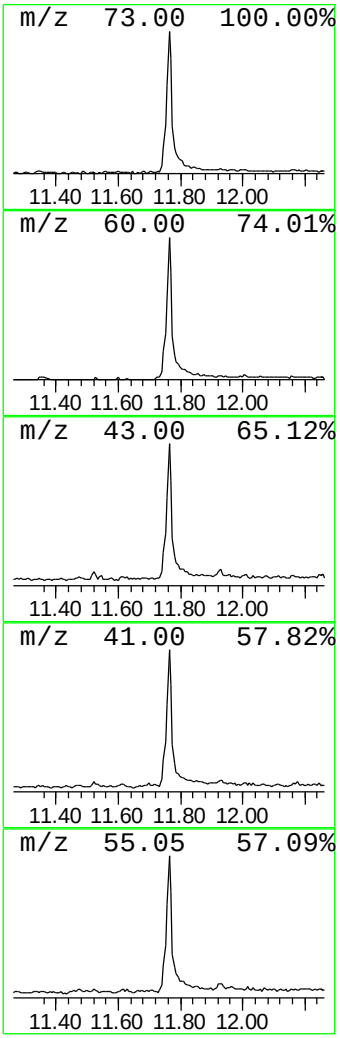
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.76	10.39 ng	519644	Phenanthrene-d10	11.23

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	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	89
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5	Undecanoic acid	186	C11H22O2	000112-37-8	64





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031120\
Data File : BF119349.D
Acq On : 11 Mar 2020 16:21
Operator : CG/JU
Sample : L1864-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1

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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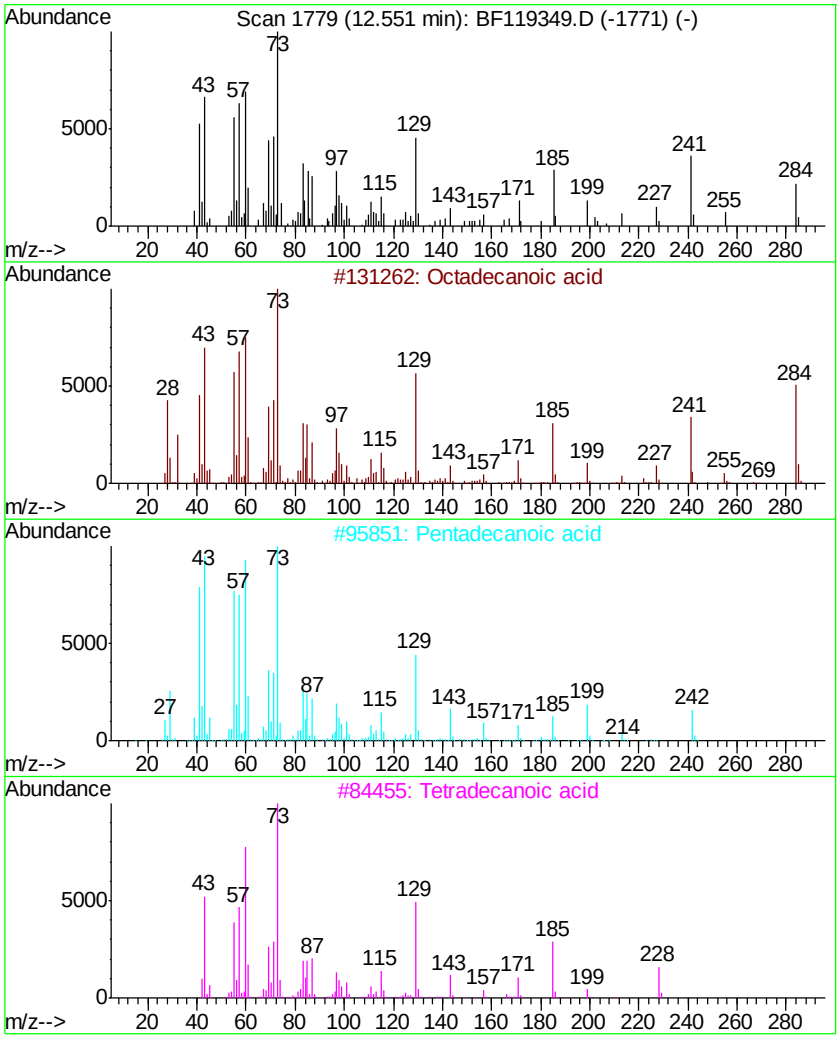
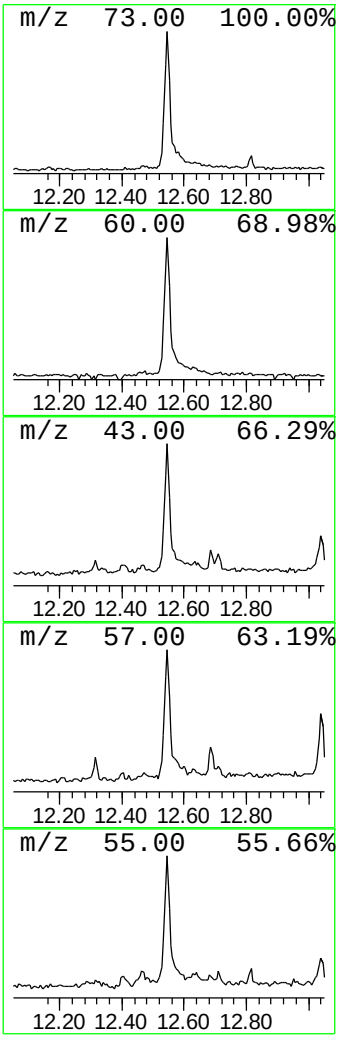
Peak Number 5 Octadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.55	6.50 ng	325263	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	58
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4	Undecanoic acid	186	C11H22O2	000112-37-8	50
5	n-Decanoic acid	172	C10H20O2	000334-48-5	50





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031120\
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Acq On : 11 Mar 2020 16:21
Operator : CG/JU
Sample : L1864-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1

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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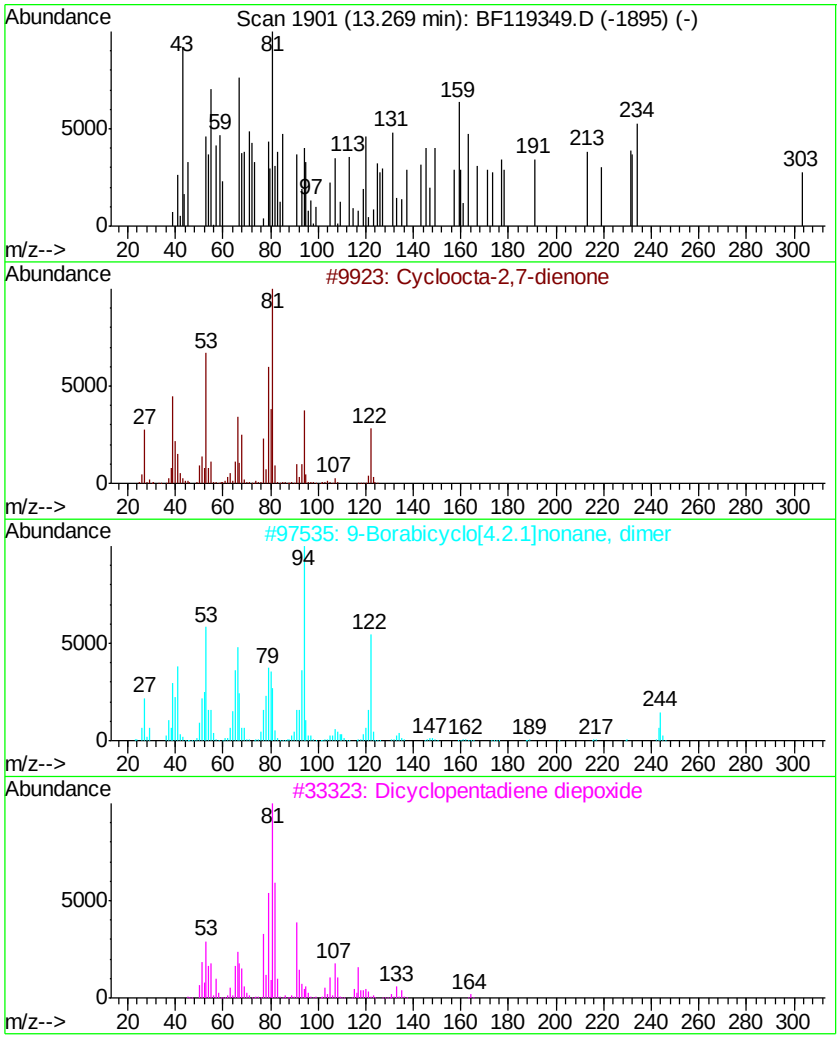
Peak Number 6 unknown13.27 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.27	2.10 ng	91390	Chrysene-d12	13.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cycloocta-2,7-dienone	122	C8H10O	1000194-03-3	38
2	9-Borabicyclo[4.2.1]nonane, dimer	244	C16H30B2	1000162-62-0	35
3	Dicyclopentadiene diepoxide	164	C10H12O2	000081-21-0	35
4	Bicyclo[2.2.1]hept-2-en-7-ol	110	C7H10O	053783-87-2	25
5	3-Heptyn-1-ol	112	C7H12O	014916-79-1	18



Library Search Compound Report

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Sample : L1864-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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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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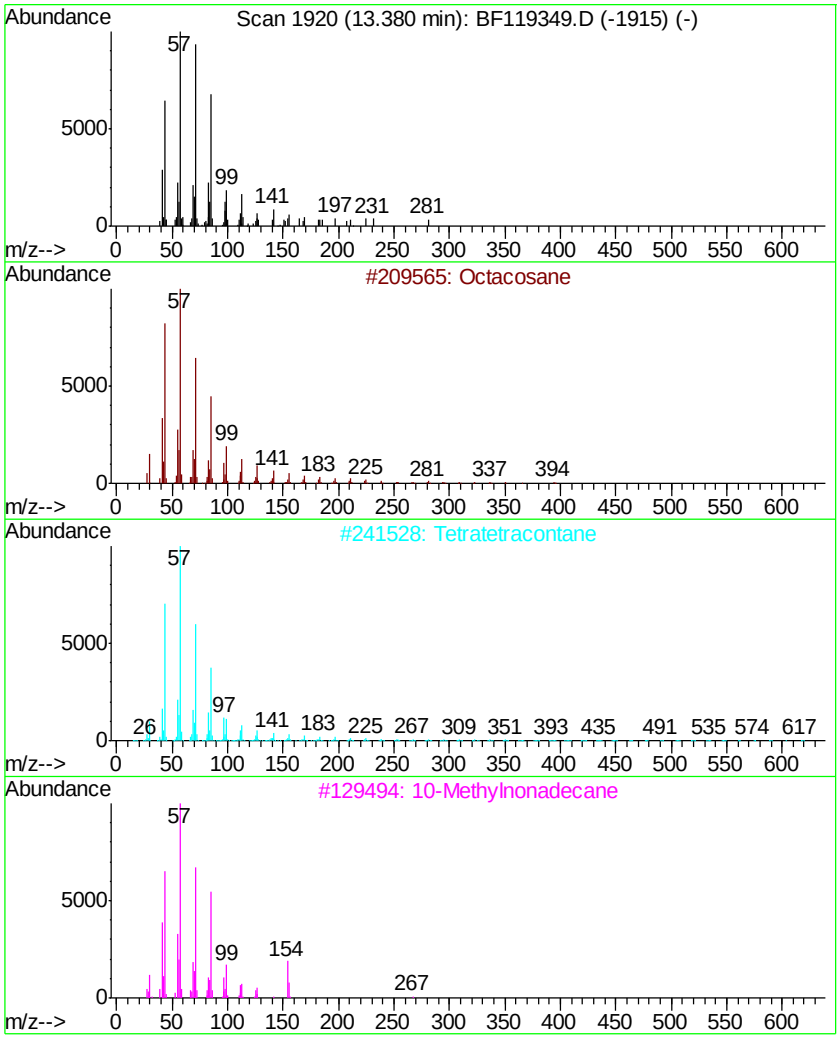
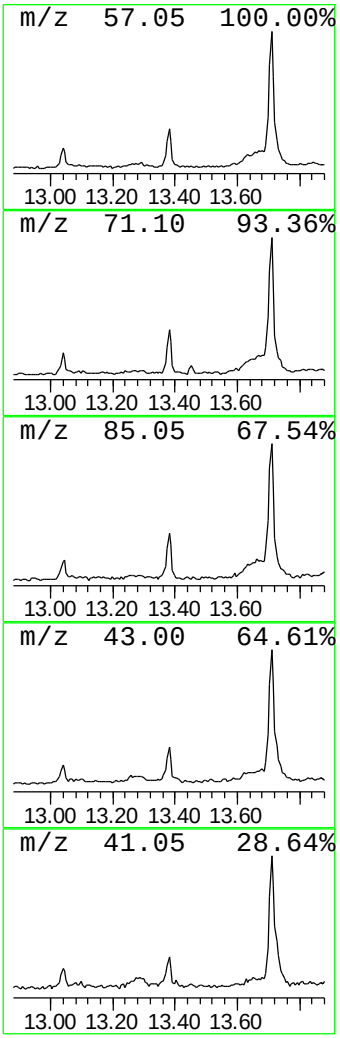
Peak Number 7 Octacosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.38	2.47 ng	107611	Chrysene-d12	13.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	86
2	Tetratetracontane	619	C44H90	007098-22-8	83
3	10-Methylnonadecane	282	C20H42	056862-62-5	80
4	2-methyloctacosane	408	C29H60	1000376-72-8	80
5	Hexacosane	366	C26H54	000630-01-3	80





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Sample : L1864-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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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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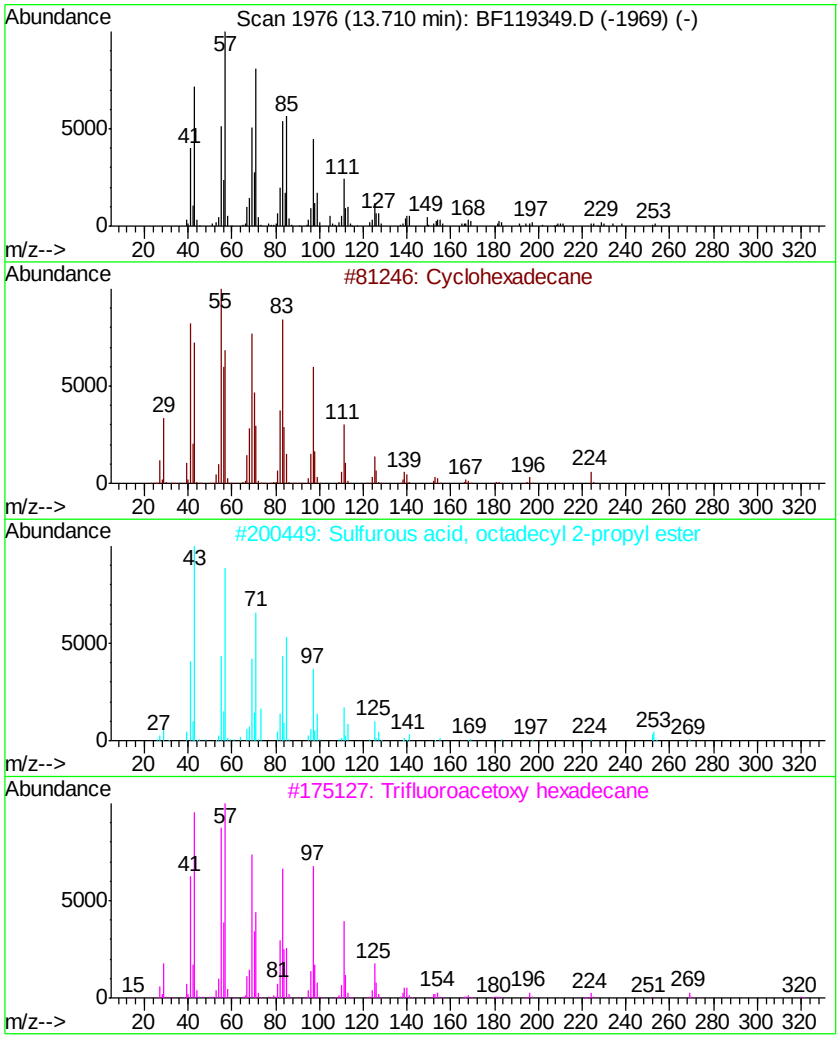
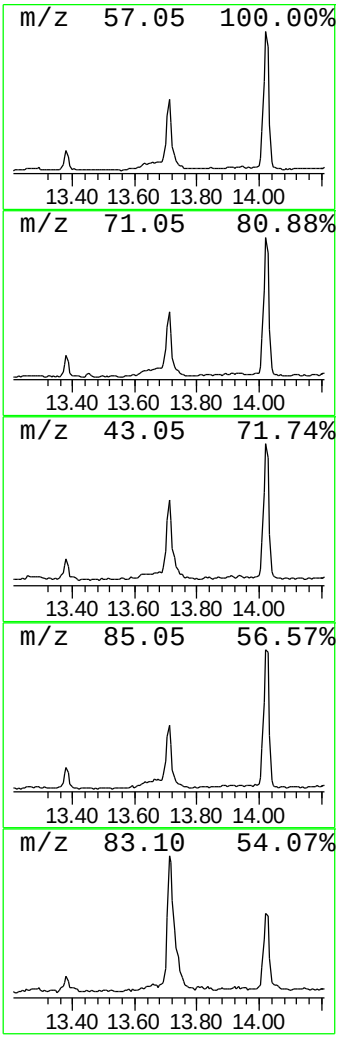
Peak Number 8 Cyclohexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.71	13.21 ng	574248	Chrysene-d12	13.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	95
2	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	91
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90
4	Cyclopentadecane	210	C15H30	000295-48-7	89
5	Cyclotetradecane	196	C14H28	000295-17-0	89





Library Search Compound Report

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BNA_F
ClientSampleId :
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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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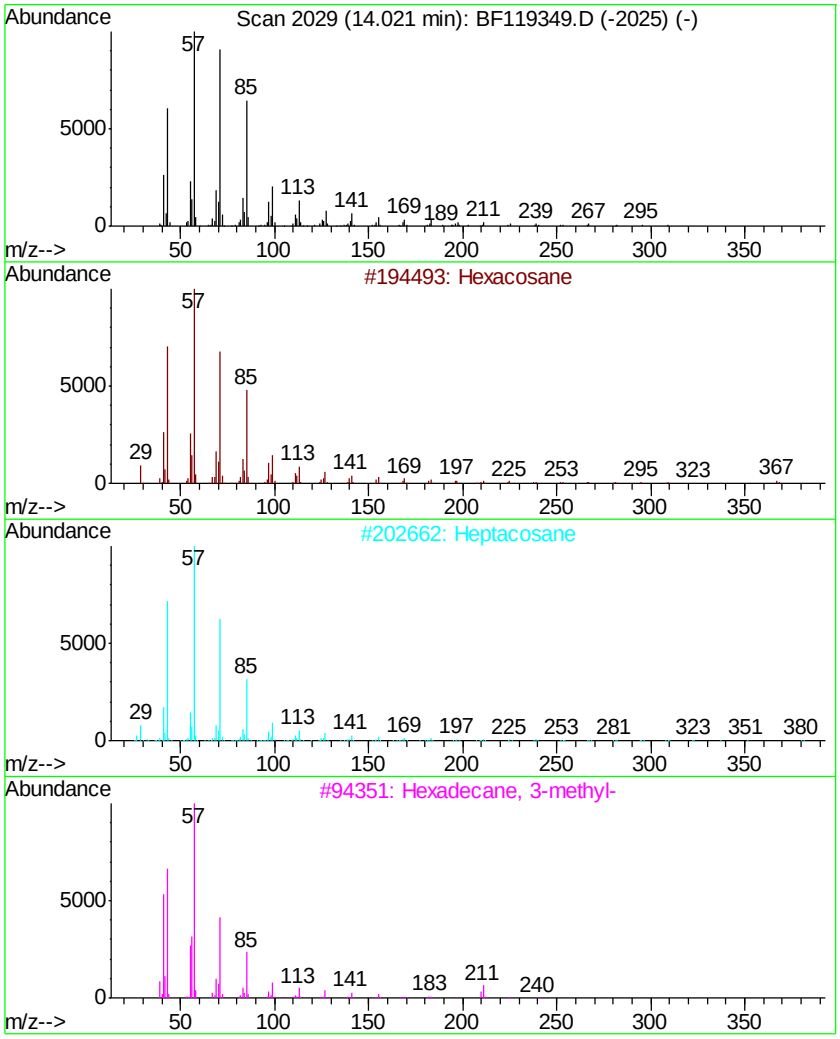
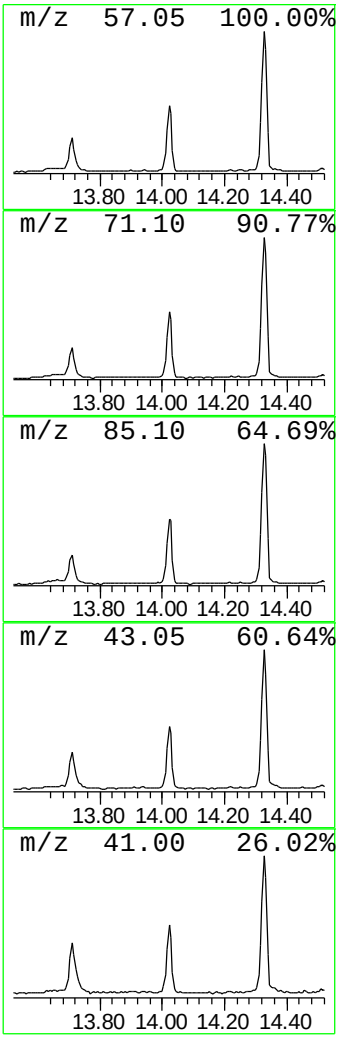
Peak Number 9 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.02	12.10 ng	526232	Chrysene-d12	13.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	94
2	Heptacosane	380	C27H56	000593-49-7	91
3	Hexadecane, 3-methyl-	240	C17H36	006418-43-5	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	2-methyloctacosane	408	C29H60	1000376-72-8	91





Library Search Compound Report

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Data File : BF119349.D
Acq On : 11 Mar 2020 16:21
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Sample : L1864-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1

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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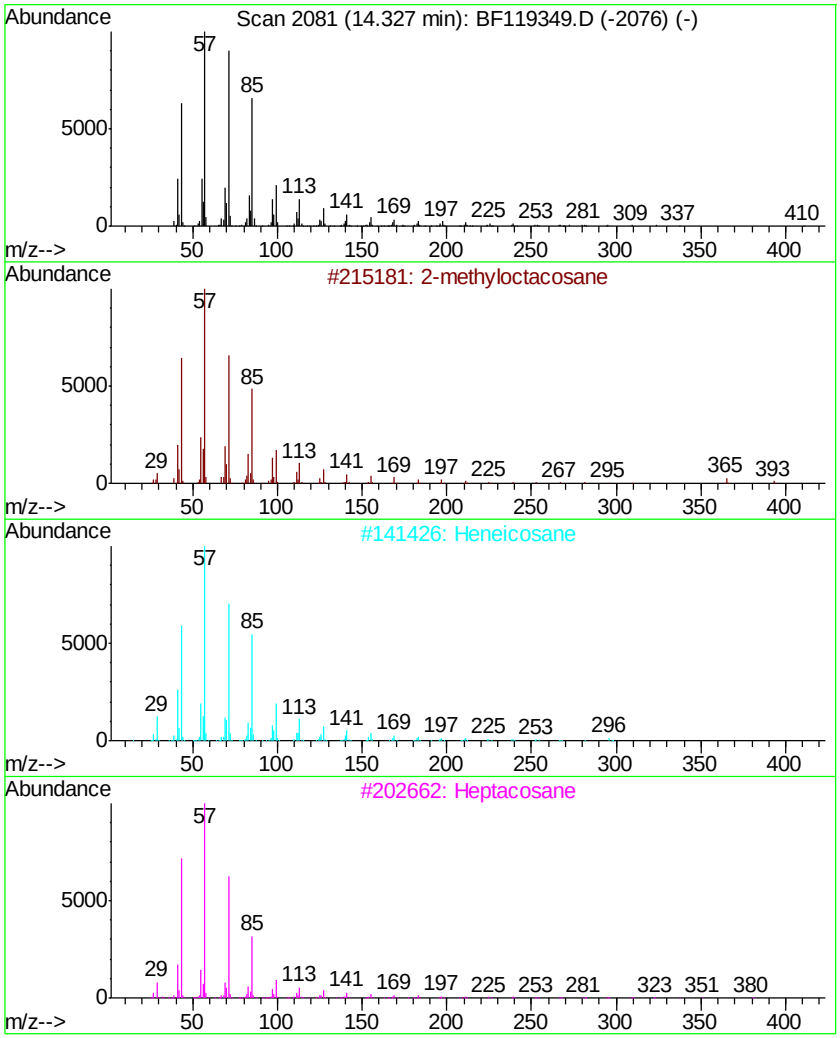
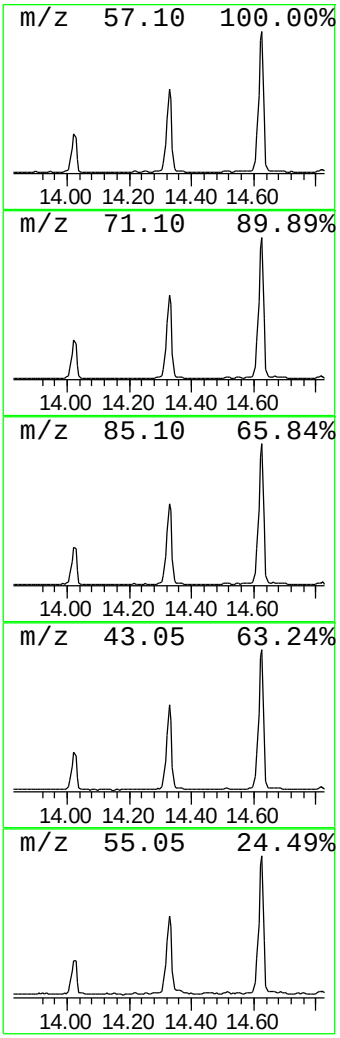
Peak Number 10 2-methyloctacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.33	26.62 ng	1157460	Chrysene-d12	13.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Heptacosane	380	C27H56	000593-49-7	91
4	Octadecane	254	C18H38	000593-45-3	91
5	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	90





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031120\
Data File : BF119349.D
Acq On : 11 Mar 2020 16:21
Operator : CG/JU
Sample : L1864-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1

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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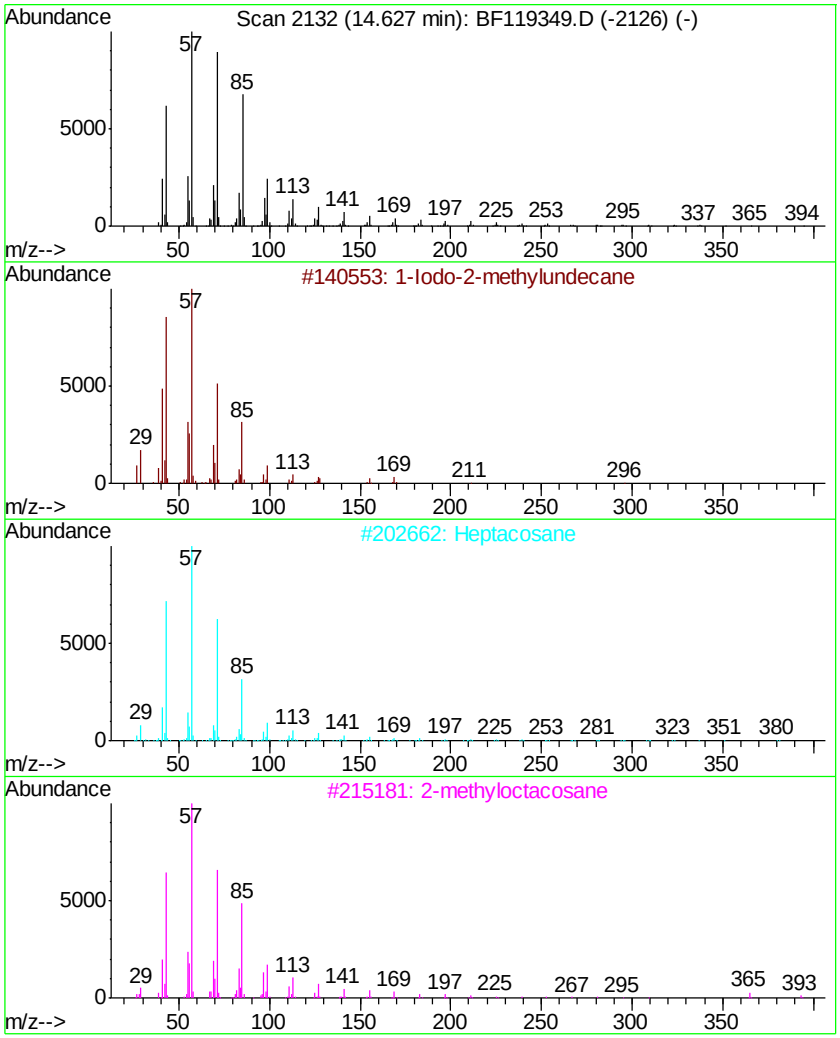
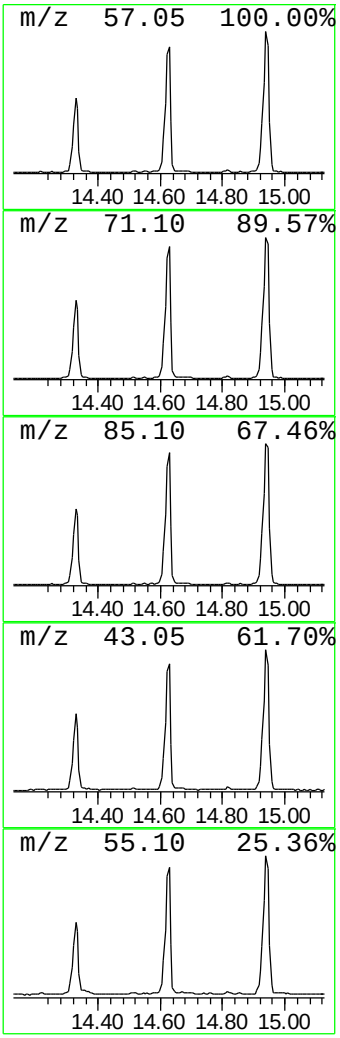
Peak Number 11 1-Iodo-2-methylundecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.63	12.53 ng	1924590	Perylene-d12	15.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	93
2	Heptacosane	380	C27H56	000593-49-7	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91





Library Search Compound Report

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Data File : BF119349.D
Acq On : 11 Mar 2020 16:21
Operator : CG/JU
Sample : L1864-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1

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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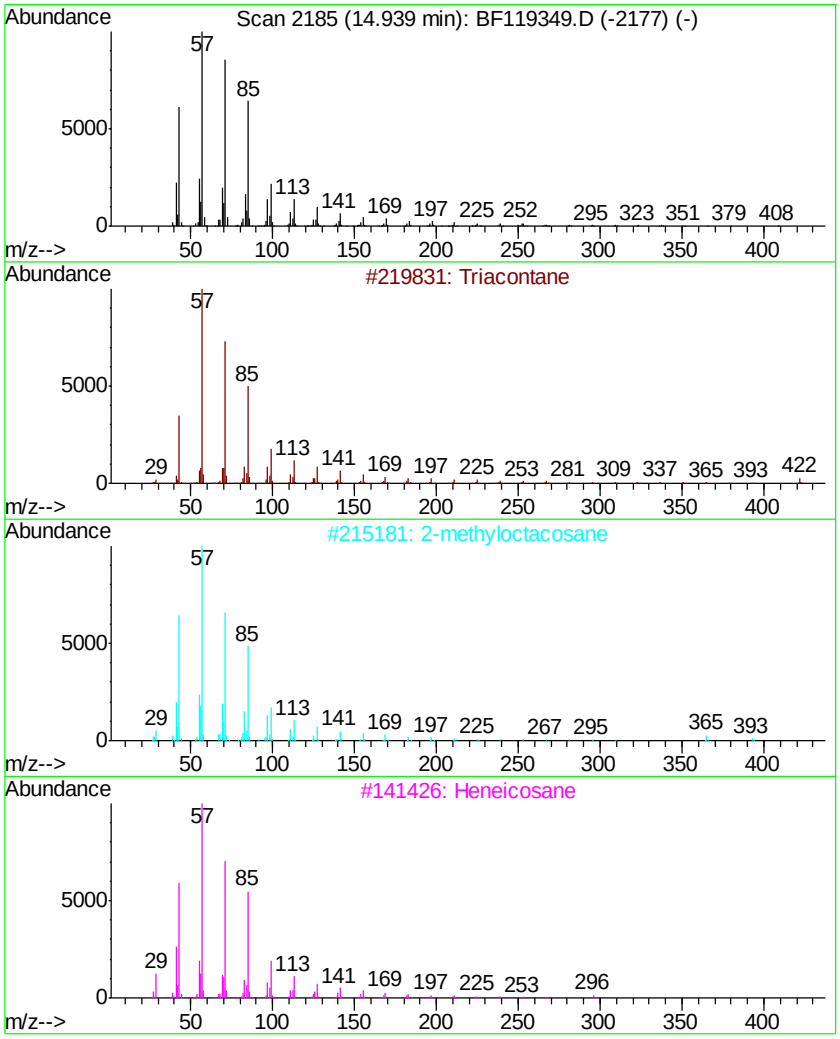
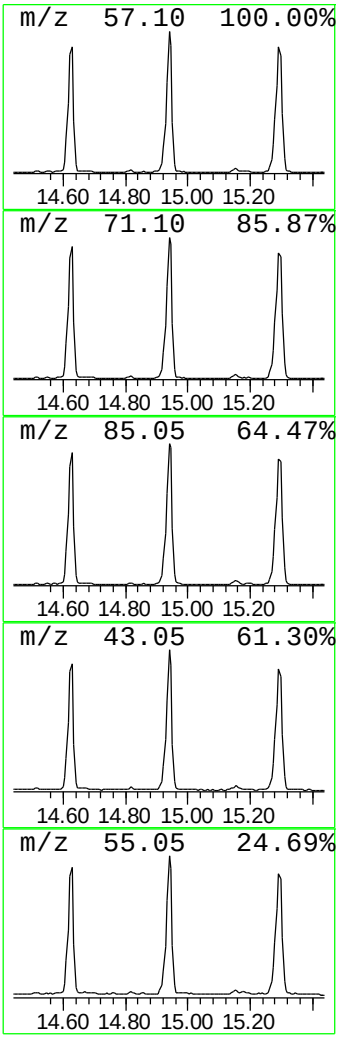
Peak Number 12 Triacontane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.94	15.65 ng	2403350	Perylene-d12	15.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Heptacosane	380	C27H56	000593-49-7	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91





Library Search Compound Report

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Data File : BF119349.D
Acq On : 11 Mar 2020 16:21
Operator : CG/JU
Sample : L1864-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1

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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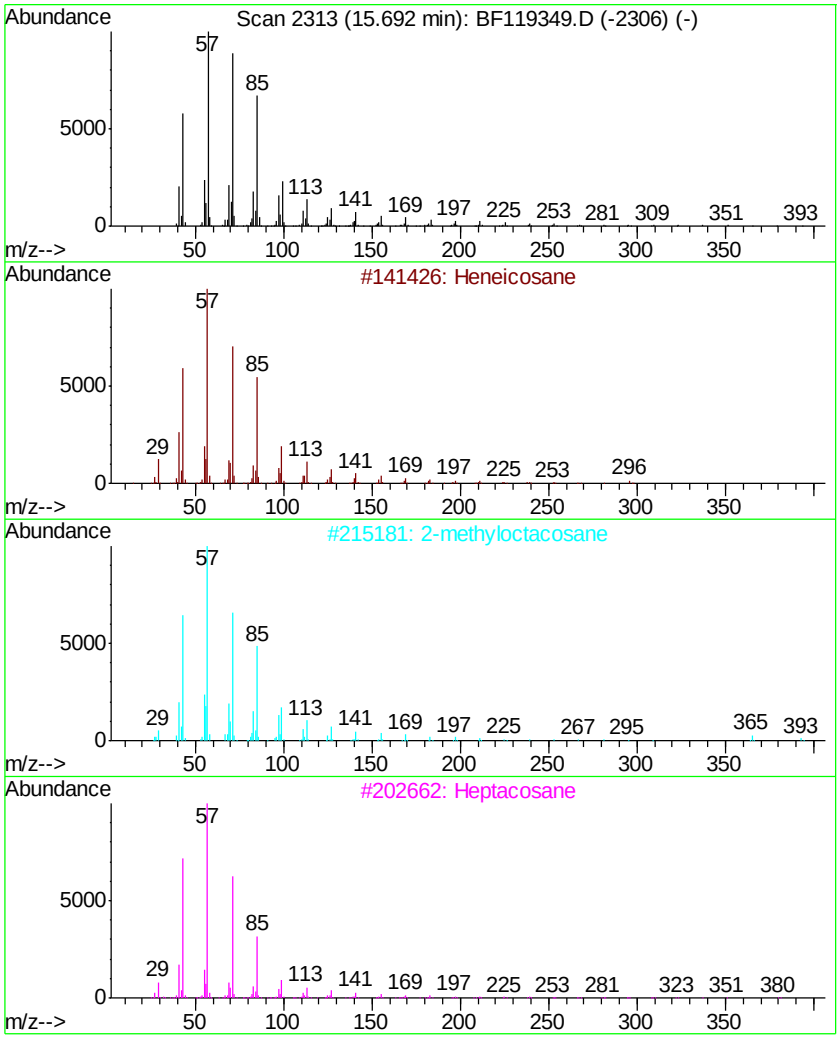
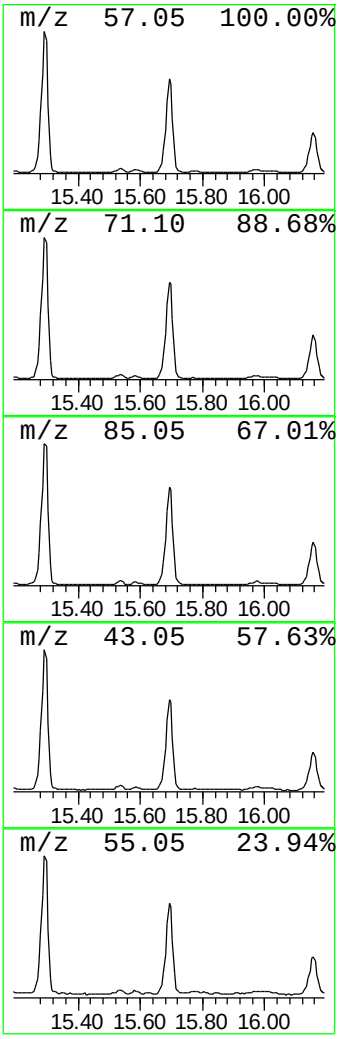
Peak Number 13 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.69	11.43 ng	1755530	Perylene-d12	15.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Heptacosane	380	C27H56	000593-49-7	91
4	Tetracosane	338	C24H50	000646-31-1	91
5	Docosane	310	C22H46	000629-97-0	91





Library Search Compound Report

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Data File : BF119349.D
Acq On : 11 Mar 2020 16:21
Operator : CG/JU
Sample : L1864-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1

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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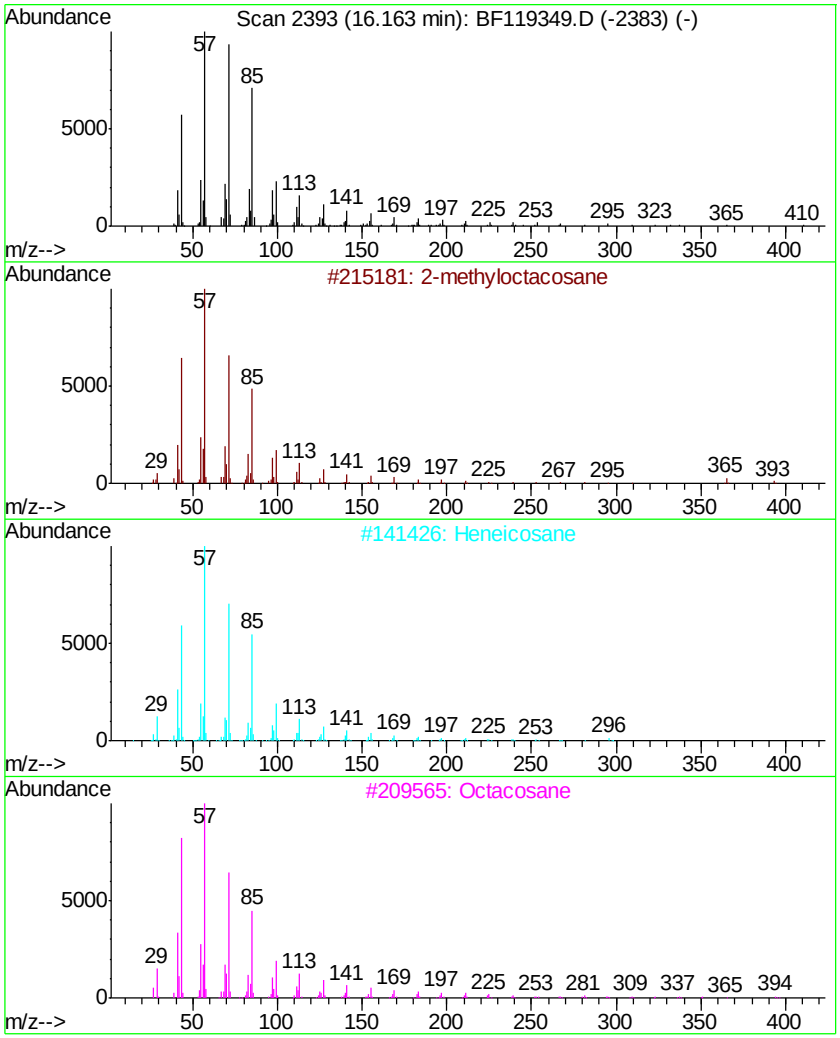
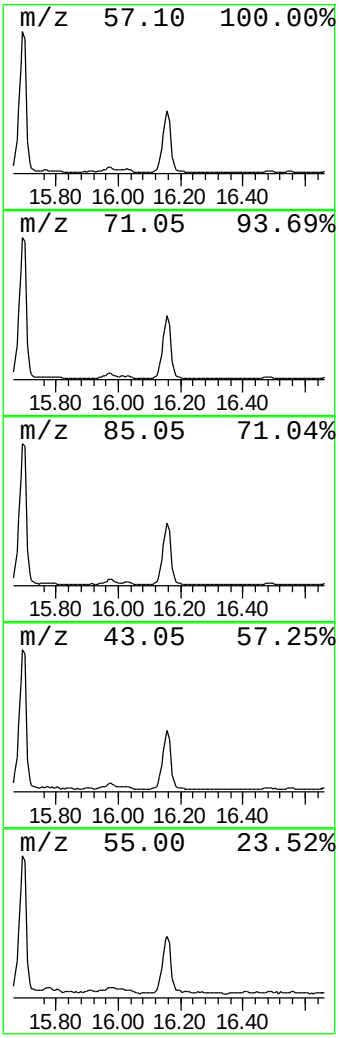
Peak Number 14 Hentriacontane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.16	6.21 ng	952895	Perylene-d12	15.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Heptacosane	380	C27H56	000593-49-7	90
5	Hentriacontane	437	C31H64	000630-04-6	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF031120\
Data File : BF119349.D
Acq On : 11 Mar 2020 16:21
Operator : CG/JU
Sample : L1864-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1

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

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
2-Pentanone, 4-hy...	4.90	8.4	ng	253803	1	6.72	604364	20.0
Phenol, 2-fluoro-	5.51	12.7	ng	382788	1	6.72	604364	20.0
n-Hexadecanoic acid	11.76	10.4	ng	519644	4	11.23	1000310	20.0
Octadecanoic acid	12.55	6.5	ng	325263	4	11.23	1000310	20.0
unknown13.27	13.27	2.1	ng	91390	5	13.88	869726	20.0
Octacosane	13.38	2.5	ng	107611	5	13.88	869726	20.0
Cyclohexadecane	13.71	13.2	ng	574248	5	13.88	869726	20.0
Hexacosane	14.02	12.1	ng	526232	5	13.88	869726	20.0
2-methyloctacosane	14.33	26.6	ng	1157460	5	13.88	869726	20.0
1-Iodo-2-methylun...	14.63	12.5	ng	1924590	6	15.31	3071110	20.0
Triacontane	14.94	15.7	ng	2403350	6	15.31	3071110	20.0
Heneicosane	15.69	11.4	ng	1755530	6	15.31	3071110	20.0
Hentriacontane	16.16	6.2	ng	952895	6	15.31	3071110	20.0