LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF123019\
Data File : BF118387.D
Acq On : 30 Dec 2019 18:09
Operator : JU
Sample : K6456-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-03

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-BF122419.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	5.057	501	505	522	rVB	347491	438728	10.28%	1.180%
2	5.469	572	575	601	rBV	2168653	2390470	56.00%	6.431%
3	6.487	744	748	767	rBV	2431075	2578126	60.39%	6.936%
4	6.622	767	771	775	rBV	3166186	2746285	64.33%	7.388%
5	6.851	806	810	817	rBV	946770	767915	17.99%	2.066%
6	7.010	833	837	848	rVB	2266164	2158257	50.56%	5.806%
7	7.416	902	906	922	rBV	1702977	1621574	37.99%	4.362%
8	8.139	1025	1029	1043	rBV	1023607	1020814	23.91%	2.746%
9	9.216	1208	1212	1223	rBV	3972409	3486667	81.68%	9.380%
10	9.616	1276	1280	1288	rVB	155140	160156	3.75%	0.431%
11	9.898	1324	1328	1333	rBV	1363372	1259555	29.51%	3.388%
12	10.698	1459	1464	1477	rBV	2375435	2493363	58.41%	6.708%
13	11.392	1578	1582	1585	rBV	1467236	1428468	33.46%	3.843%
14	11.416	1585	1586	1591	rVV	433772	313867	7.35%	0.844%
15	11.469	1591	1595	1599	rVB2	55870	89041	2.09%	0.240%
16	11.633	1618	1623	1628	rBV4	29620	54778	1.28%	0.147%
17	11.916	1665	1671	1678	rBV2	375682	516011	12.09%	1.388%
18	12.010	1684	1687	1690	rBV2	83640	93613	2.19%	0.252%
19	12.451	1758	1762	1764	rBV	61375	66456	1.56%	0.179%
20	12.545	1774	1778	1781	rVB3	35981	47558	1.11%	0.128%
21	12.616	1786	1790	1795	rBV	658476	647072	15.16%	1.741%
22	12.704	1802	1805	1810	rBV2	92164	99508	2.33%	0.268%
23	12.845	1823	1829	1835	rBV	634336	689549	16.15%	1.855%
24	12.986	1844	1853	1856	rBV	4843603	4268811	100.00%	11.484%
25	13.069	1861	1867	1871	rVB3	46112	83647	1.96%	0.225%
26	13.151	1877	1881	1883	rBV4	47284	64168	1.50%	0.173%
27	13.280	1898	1903	1910	rVB2	61442	90641	2.12%	0.244%
28	13.545	1943	1948	1951	rBV2	85762	92172	2.16%	0.248%
29	13.692	1970	1973	1976	rBV	56615	49790	1.17%	0.134%
30	13.798	1986	1991	1993	rBV	58870	64038	1.50%	0.172%
31	13.874	2001	2004	2015	rVB3	494240	708462	16.60%	1.906%
32	14.051	2028	2034	2036	rBV2	1324978	1460568	34.21%	3.929%
33	14.074	2036	2038	2042	rVB	277105	225040	5.27%	0.605%
34	14.192	2055	2058	2062	rBV	263236	255458	5.98%	0.687%

LSC Area Percent Report

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Operator : JU
Sample : K6456-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-03

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-BF122419.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.439	2095	2100	2103	rVB	59453	60856	1.43%	0.164%
36	14.498	2107	2110	2119	rVV	386493	413319	9.68%	1.112%
37	14.810	2158	2163	2167	rBV	448064	434584	10.18%	1.169%
38	15.104	2209	2213	2216	rBV	213566	307954	7.21%	0.828%
39	15.151	2218	2221	2226	rVV	419806	478133	11.20%	1.286%
40	15.215	2229	2232	2236	rVB	43335	54279	1.27%	0.146%
41	15.410	2262	2265	2272	rVB	116641	146174	3.42%	0.393%
42	15.474	2272	2276	2282	rVV	174570	223440	5.23%	0.601%
43	15.539	2282	2287	2299	rVB2	1072089	1487468	34.85%	4.002%
44	15.980	2356	2362	2369	rBV	238747	363096	8.51%	0.977%
45	16.045	2369	2373	2382	rBV	43407	121992	2.86%	0.328%
46	16.492	2443	2449	2455	rBV	125862	218688	5.12%	0.588%
47	17.051	2539	2544	2549	rBV	73771	166940	3.91%	0.449%
48	17.233	2570	2575	2582	rBV6	20305	52499	1.23%	0.141%
49	17.509	2617	2622	2631	rBV	52621	111665	2.62%	0.300%

Sum of corrected areas: 37171713

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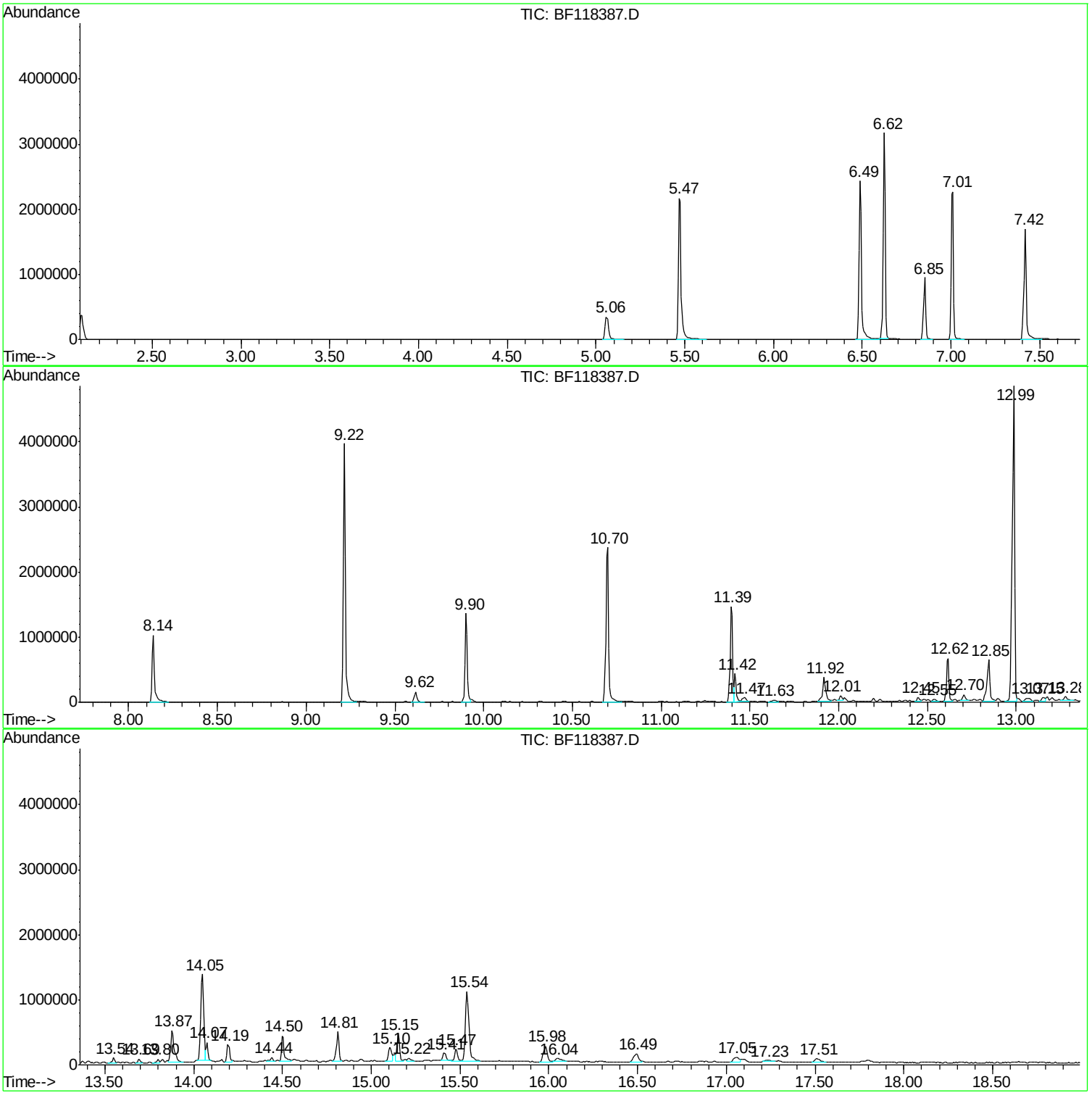
Instrument :
BNA_F
ClientSampleId :
SB-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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 : BF118387.D
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Operator : JU
Sample : K6456-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

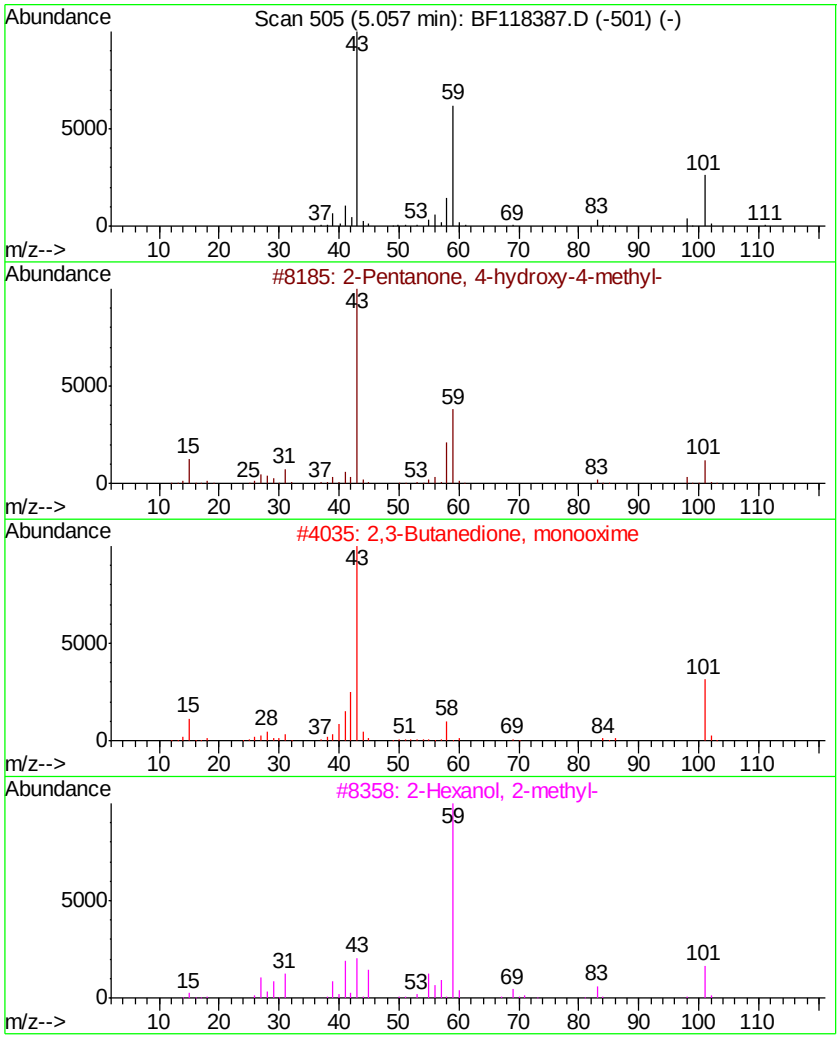
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

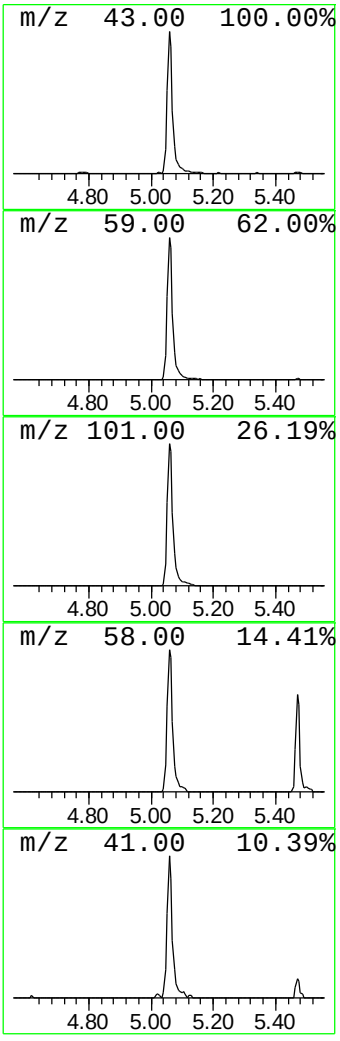
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	11.43 ng	438728	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	23
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF123019\
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Acq On : 30 Dec 2019 18:09
Operator : JU
Sample : K6456-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

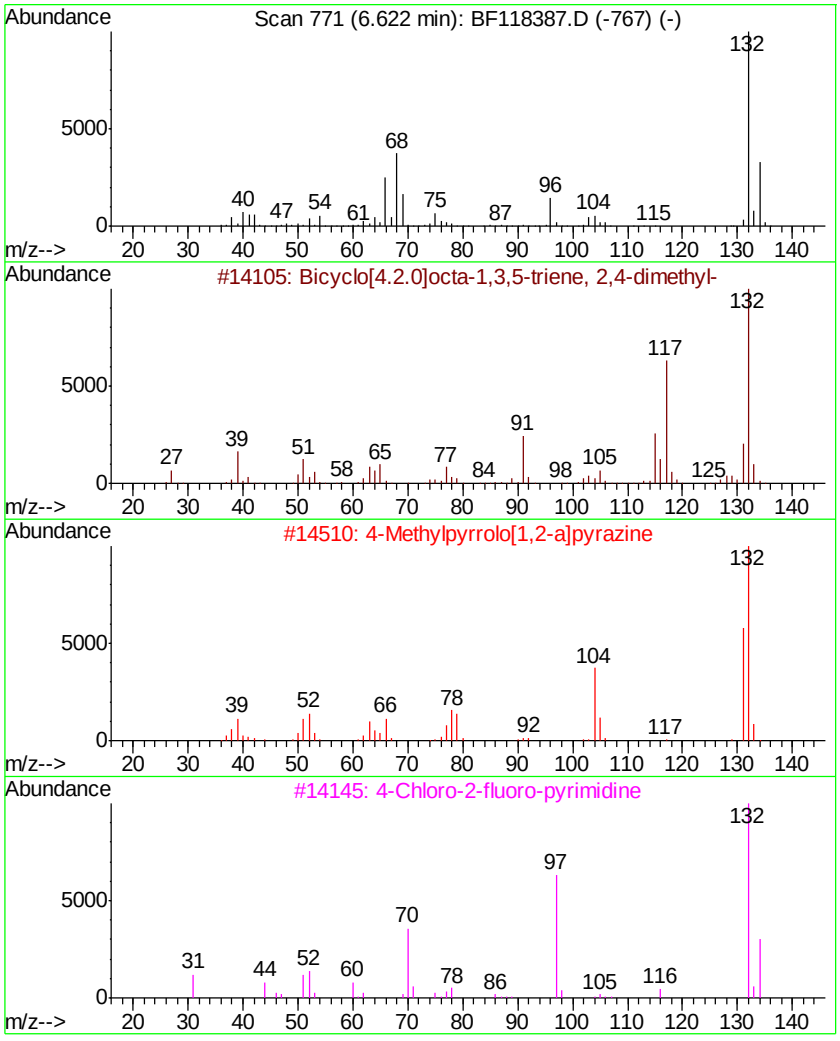
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

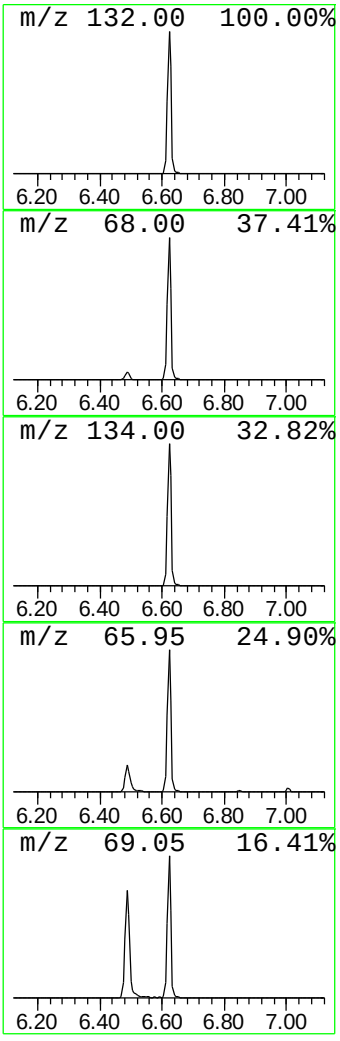
****

Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	71.53 ng	2746290	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
2	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF123019\
Data File : BF118387.D
Acq On : 30 Dec 2019 18:09
Operator : JU
Sample : K6456-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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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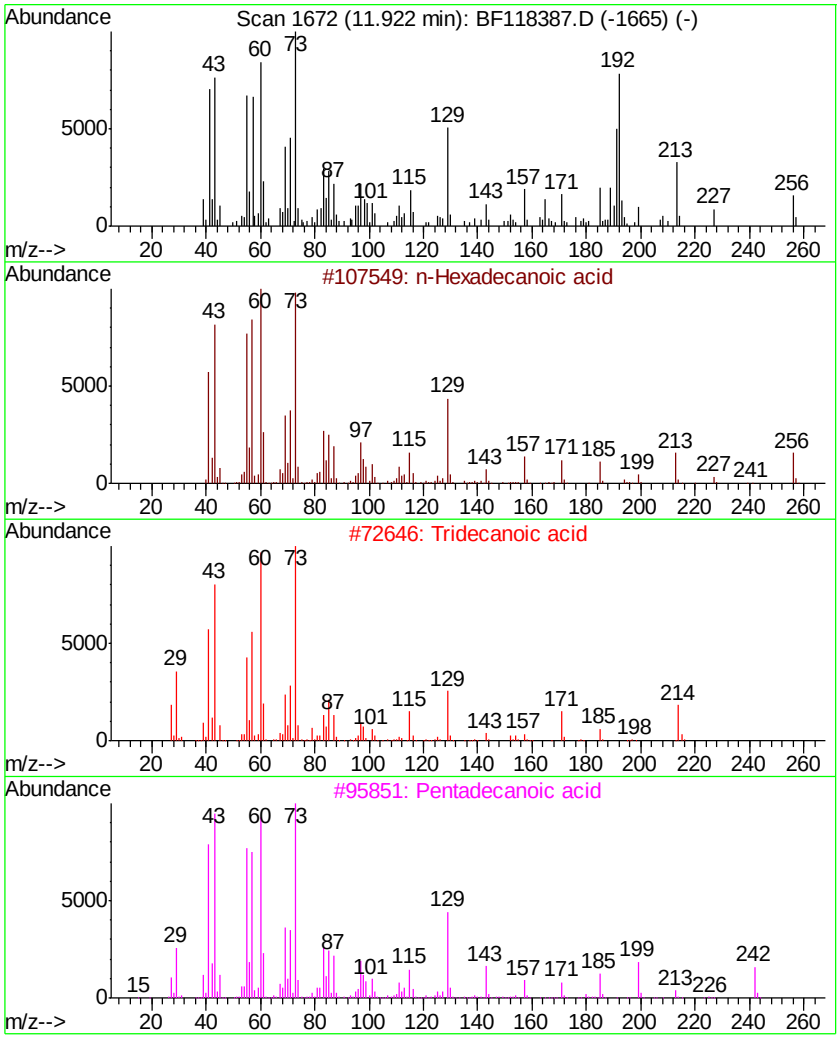
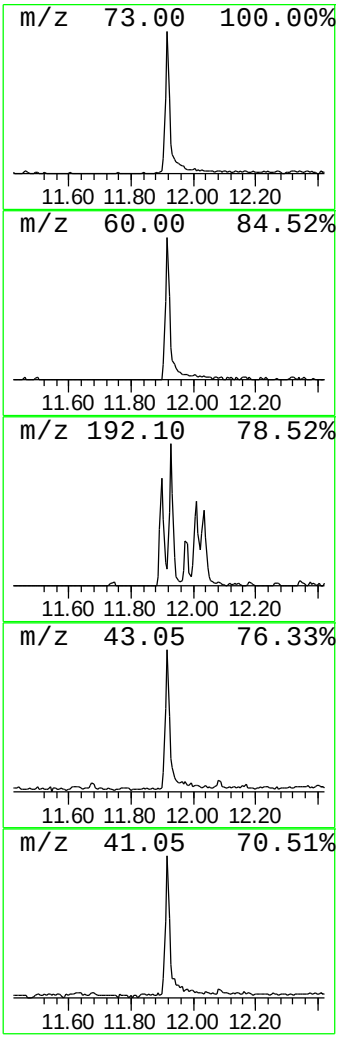
Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	7.22 ng	516011	Phenanthrene-d10	11.39

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	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Undecanoic acid	186	C11H22O2	000112-37-8	74





Library Search Compound Report

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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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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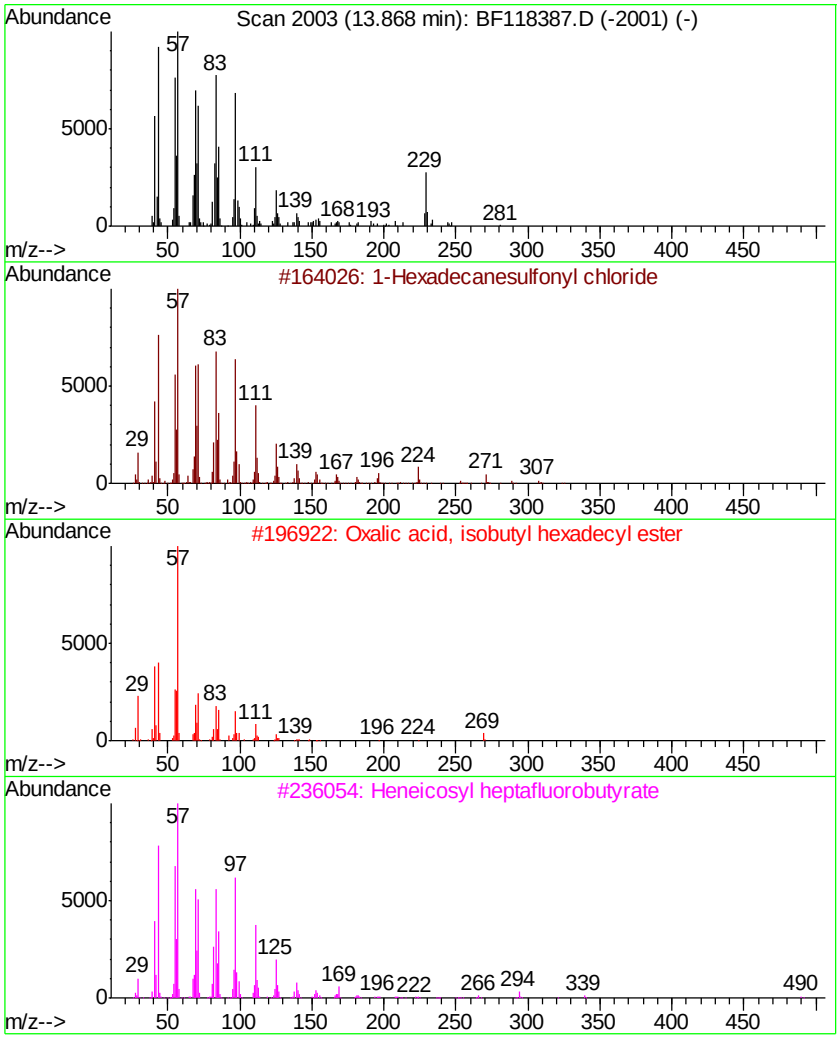
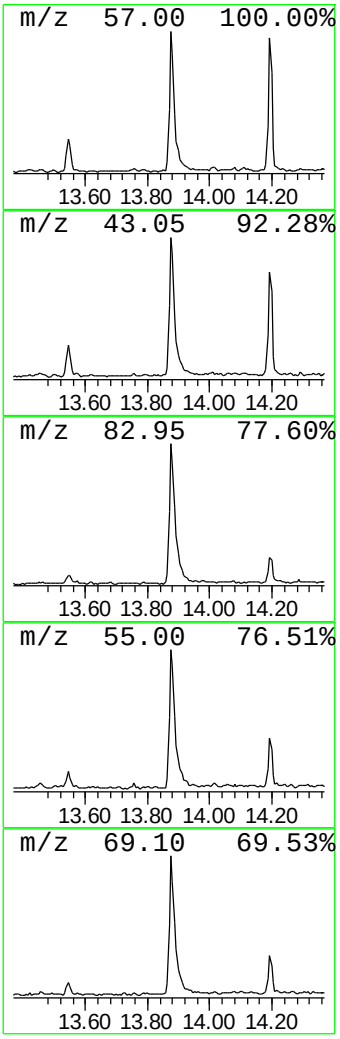
Peak Number 5 1-Hexadecanesulfonyl chloride Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	9.70 ng	708462	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	91
2	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
3	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	90
4	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	87
5	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	87





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Instrument : BNA_F
ClientSampleId : SB-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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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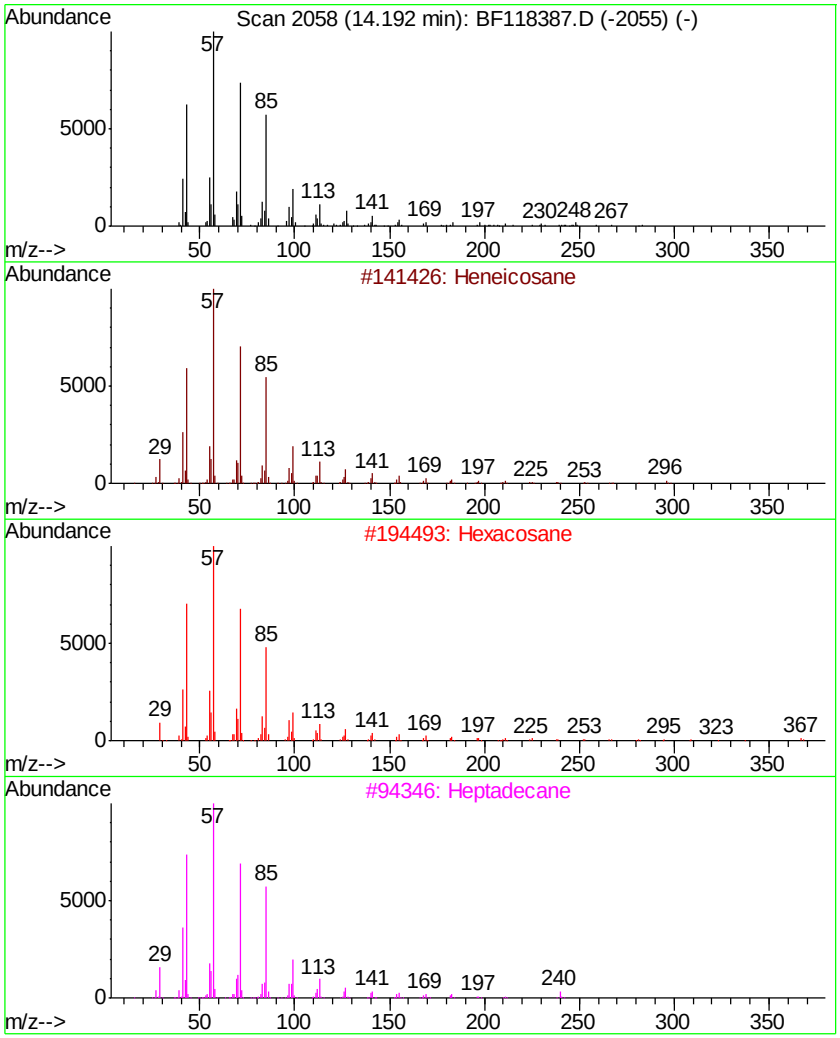
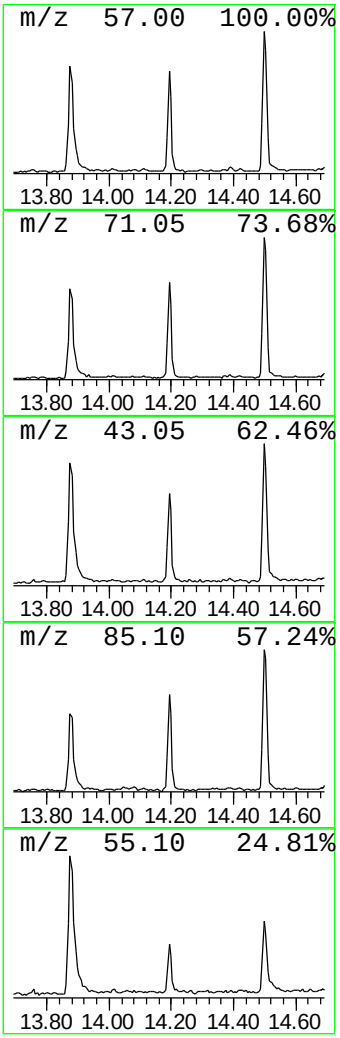
Peak Number 6 Heptadecane, 9-octyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.19	3.50 ng	255458	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Heptadecane	240	C17H36	000629-78-7	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90





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Data File : BF118387.D
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Misc :
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Instrument : BNA_F
ClientSampleId : SB-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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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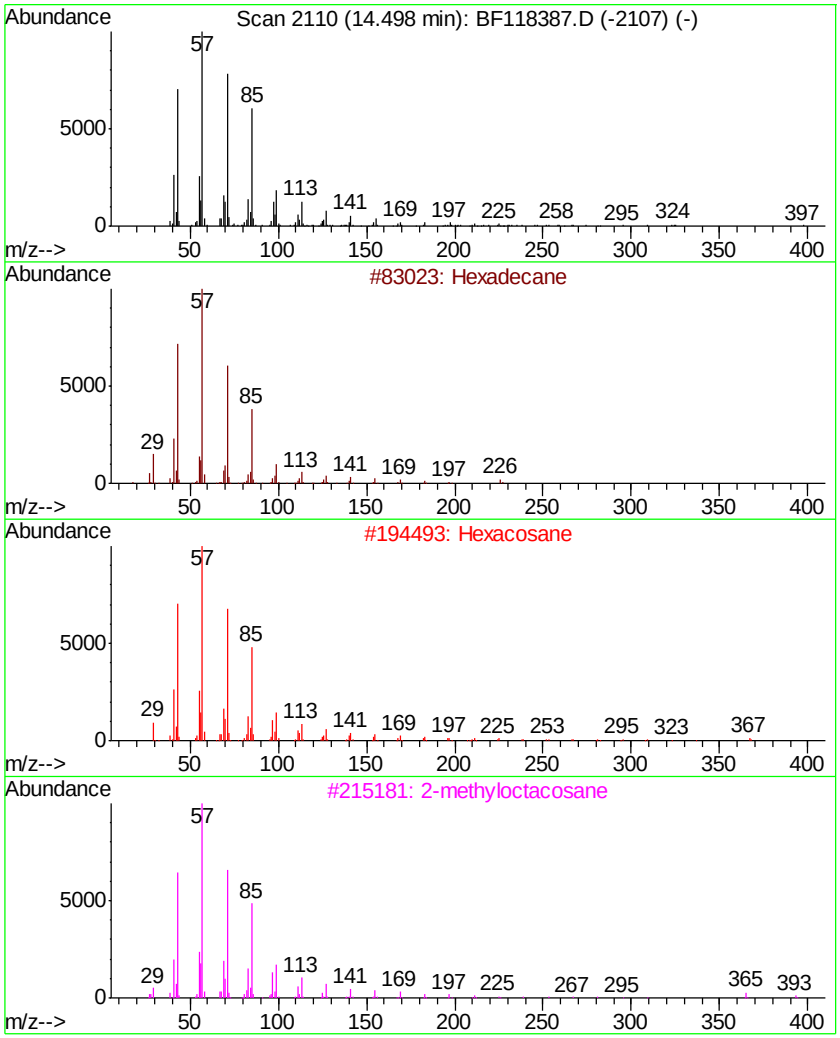
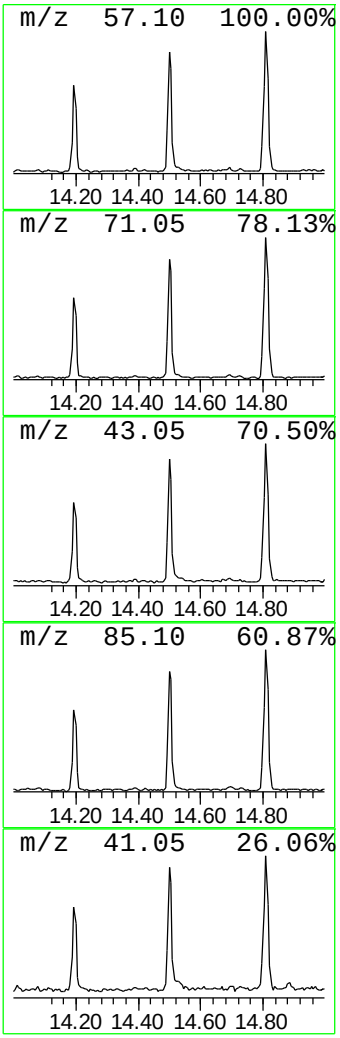
Peak Number 7 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.50	5.66 ng	413319	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	95
2	Hexacosane	366	C26H54	000630-01-3	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91





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Misc :
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Instrument : BNA_F
ClientSampleId : SB-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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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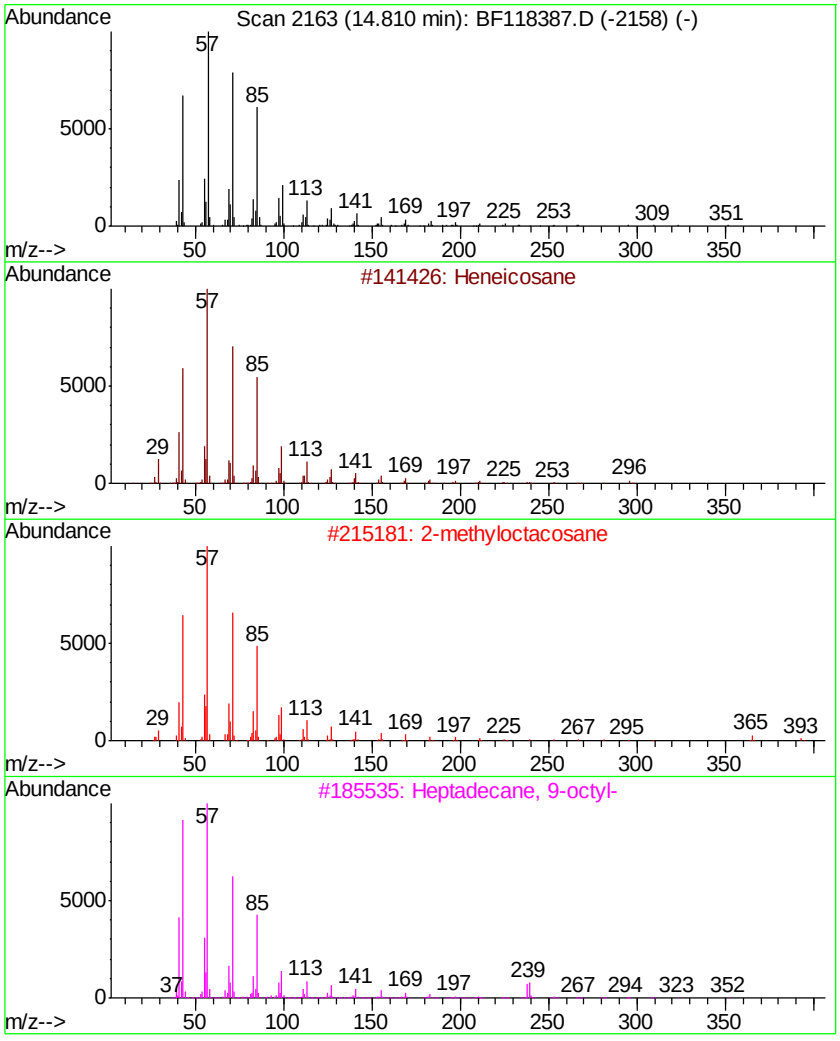
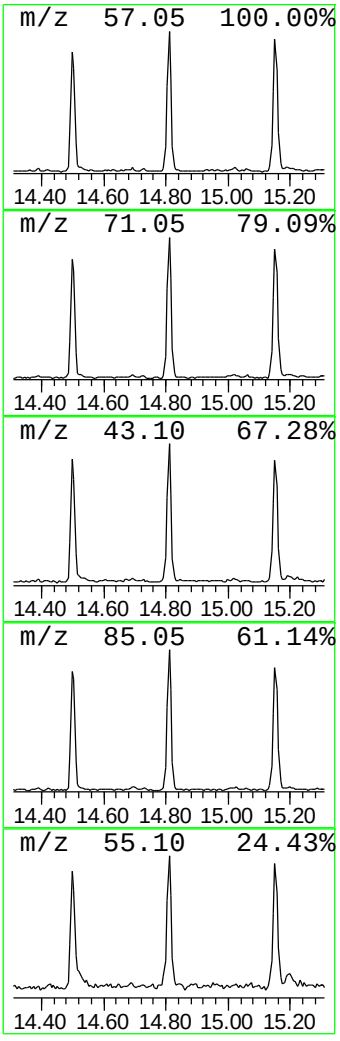
Peak Number 8 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.81	5.84 ng	434584	Perylene-d12	15.54

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	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
5	Octacosane	394	C28H58	000630-02-4	90





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF123019\
Data File : BF118387.D
Acq On : 30 Dec 2019 18:09
Operator : JU
Sample : K6456-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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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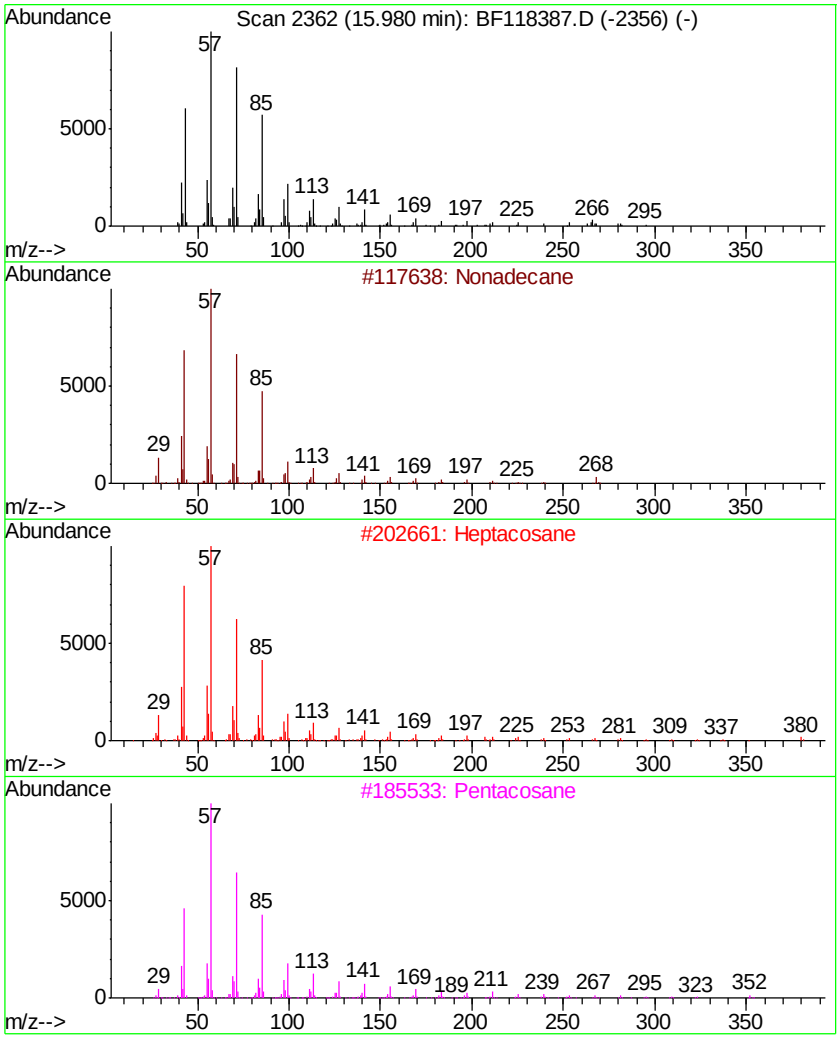
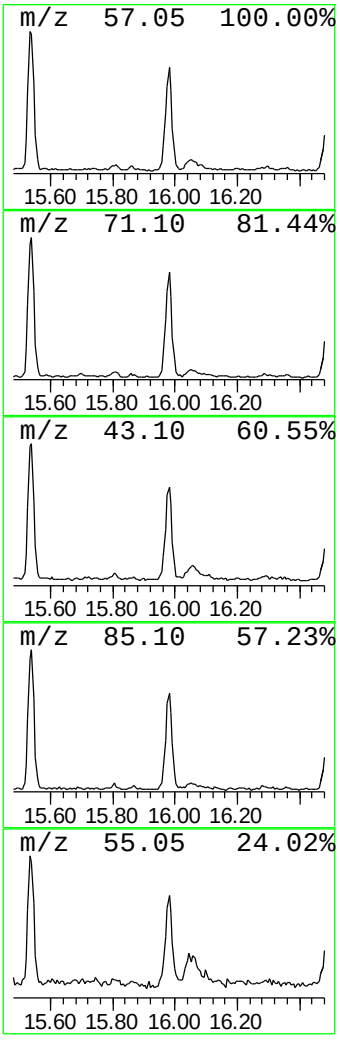
Peak Number 9 Nonadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.98	4.88 ng	363096	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	93
2	Heptacosane	380	C27H56	000593-49-7	91
3	Pentacosane	352	C25H52	000629-99-2	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Heneicosane	296	C21H44	000629-94-7	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF123019\
Data File : BF118387.D
Acq On : 30 Dec 2019 18:09
Operator : JU
Sample : K6456-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

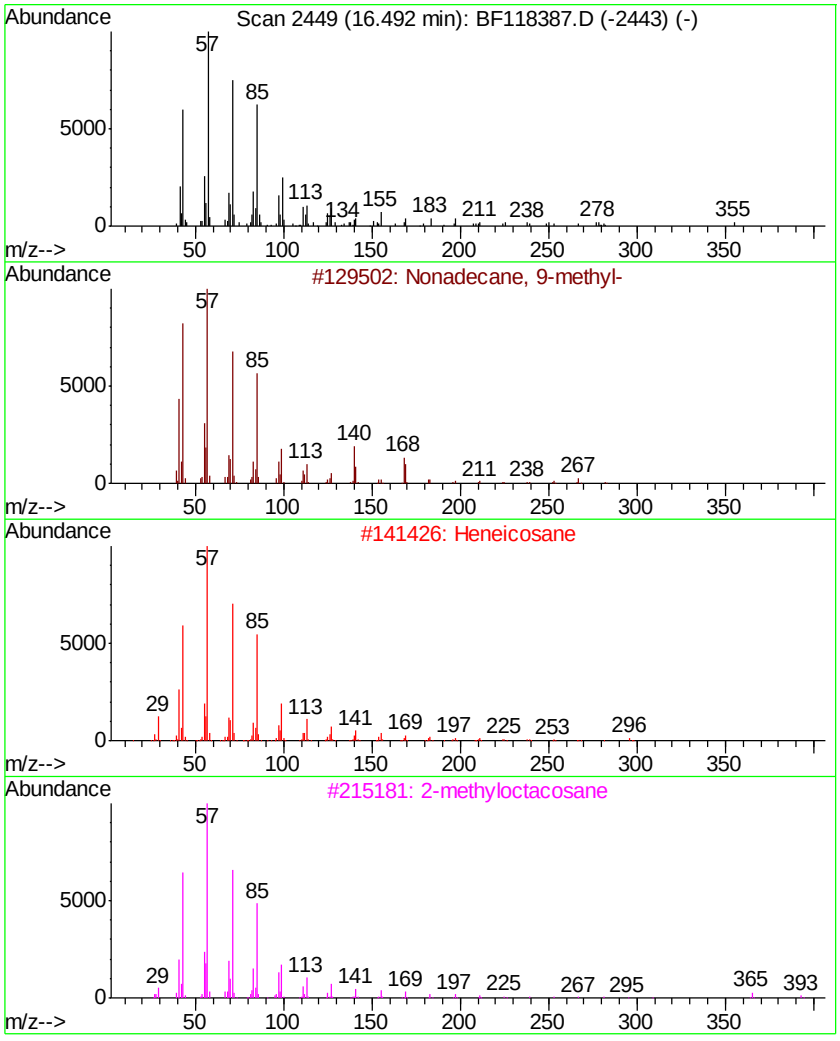
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

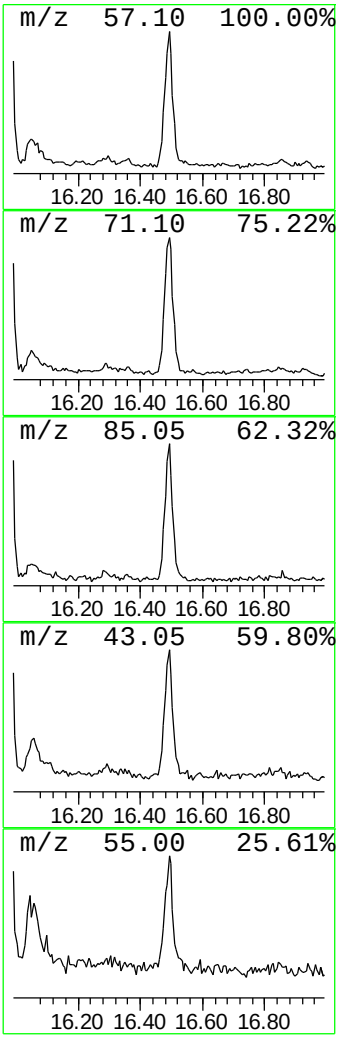
****

Peak Number 10 Nonadecane, 9-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.49	2.94 ng	218688	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	93
2	Heneicosane	296	C21H44	000629-94-7	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Tetracosane	338	C24H50	000646-31-1	90
5	Eicosane	282	C20H42	000112-95-8	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF123019\
Data File : BF118387.D
Acq On : 30 Dec 2019 18:09
Operator : JU
Sample : K6456-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-03

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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
2-Pentanone, 4-hy...	5.06	11.4	ng	438728	1	6.85	767915	20.0
unknown6.62	6.62	71.5	ng	2746290	1	6.85	767915	20.0
n-Hexadecanoic acid	11.92	7.2	ng	516011	4	11.39	1428470	20.0
1-Hexadecanesulfo...	13.87	9.7	ng	708462	5	14.05	1460570	20.0
Heptadecane, 9-oc...	14.19	3.5	ng	255458	5	14.05	1460570	20.0
Hexadecane	14.50	5.7	ng	413319	5	14.05	1460570	20.0
Heneicosane	14.81	5.8	ng	434584	6	15.54	1487470	20.0
Nonadecane	15.98	4.9	ng	363096	6	15.54	1487470	20.0
Nonadecane, 9-met...	16.49	2.9	ng	218688	6	15.54	1487470	20.0