LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101019\
Data File : BF117365.D
Acq On : 10 Oct 2019 17:35
Operator : JU
Sample : K5297-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

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-BF091319.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	5.004	492	496	507	rBV	40563	60204	6.00%	0.551%
2	5.422	563	567	587	rBV	701686	856005	85.27%	7.830%
3	6.439	736	740	758	rBV	915122	984741	98.10%	9.008%
4	6.569	758	762	777	rVB	1152721	1003855	100.00%	9.183%
5	6.792	797	800	812	rVB	264787	250317	24.94%	2.290%
6	6.951	823	827	842	rBV	715829	674246	67.17%	6.168%
7	7.357	892	896	922	rBV	470253	586645	58.44%	5.366%
8	8.075	1015	1018	1038	rBV	239149	320469	31.92%	2.932%
9	9.151	1197	1201	1213	rBV	1014864	967334	96.36%	8.849%
10	9.545	1265	1268	1282	rBV	155390	149506	14.89%	1.368%
11	9.827	1313	1316	1328	rBV	382265	394221	39.27%	3.606%
12	10.380	1407	1410	1415	rVB	10258	11886	1.18%	0.109%
13	10.621	1447	1451	1462	rBV	619753	627202	62.48%	5.737%
14	11.316	1566	1569	1572	rBV	378093	375414	37.40%	3.434%
15	11.339	1572	1573	1578	rVV	102575	82435	8.21%	0.754%
16	11.398	1578	1583	1587	rVB	23778	31383	3.13%	0.287%
17	11.821	1652	1655	1656	rBV	17876	15596	1.55%	0.143%
18	11.839	1656	1658	1666	rVB3	63216	84172	8.38%	0.770%
19	11.933	1671	1674	1677	rBV	44173	45232	4.51%	0.414%
20	12.116	1702	1705	1709	rVB	14673	13573	1.35%	0.124%
21	12.368	1745	1748	1751	rBV	14928	16128	1.61%	0.148%
22	12.533	1773	1776	1781	rBV	313952	275144	27.41%	2.517%
23	12.627	1789	1792	1798	rBV3	11805	16814	1.67%	0.154%
24	12.686	1798	1802	1808	rVB4	10408	14514	1.45%	0.133%
25	12.763	1809	1815	1821	rBV	234537	261591	26.06%	2.393%
26	12.815	1821	1824	1831	rVB2	10613	13850	1.38%	0.127%
27	12.898	1834	1838	1841	rBV	993331	822621	81.95%	7.525%
28	12.974	1848	1851	1857	rVB2	15726	25452	2.54%	0.233%
29	13.092	1864	1871	1874	rBV2	44051	60266	6.00%	0.551%
30	13.157	1880	1882	1885	rVB	36554	29879	2.98%	0.273%
31	13.198	1885	1889	1896	rBV4	19378	28133	2.80%	0.257%
32	13.292	1901	1905	1907	rBV	12962	14573	1.45%	0.133%
33	13.321	1907	1910	1916	rBV	10069	13634	1.36%	0.125%
34	13.468	1930	1935	1937	rBV4	8293	11629	1.16%	0.106%

LSC Area Percent Report

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Acq On : 10 Oct 2019 17:35
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Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

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-BF091319.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.580	1949	1954	1957	rBV4	7780	11949	1.19%	0.109%
36	13.715	1974	1977	1978	rBV	18448	14469	1.44%	0.132%
37	13.733	1978	1980	1983	rVV2	17523	16673	1.66%	0.153%
38	13.792	1987	1990	2001	rVB5	83748	155740	15.51%	1.425%
39	13.927	2010	2013	2014	rBV	20894	18268	1.82%	0.167%
40	13.962	2014	2019	2021	rVV2	293081	371974	37.05%	3.403%
41	13.986	2021	2023	2031	rVB	97441	102786	10.24%	0.940%
42	14.068	2034	2037	2040	rVB	13587	11339	1.13%	0.104%
43	14.109	2041	2044	2048	rBV3	16672	19791	1.97%	0.181%
44	14.351	2081	2085	2089	rBV2	18054	24989	2.49%	0.229%
45	14.415	2094	2096	2098	rBV	34671	27368	2.73%	0.250%
46	14.698	2141	2144	2145	rBV	40766	35339	3.52%	0.323%
47	14.715	2145	2147	2150	rVB	50579	46028	4.59%	0.421%
48	14.851	2167	2170	2173	rVB5	12615	13756	1.37%	0.126%
49	15.004	2191	2196	2198	rBV	75458	106688	10.63%	0.976%
50	15.045	2200	2203	2207	rVV	67140	80304	8.00%	0.735%
51	15.109	2211	2214	2218	rVB3	18773	23795	2.37%	0.218%
52	15.298	2243	2246	2251	rVB	42780	50507	5.03%	0.462%
53	15.362	2252	2257	2261	rBV	57151	74126	7.38%	0.678%
54	15.415	2261	2266	2271	rBV2	214579	303940	30.28%	2.780%
55	15.827	2332	2336	2341	rBV	49656	71304	7.10%	0.652%
56	16.315	2414	2419	2424	rBV	25874	41228	4.11%	0.377%
57	16.727	2484	2489	2492	rVB5	8129	13722	1.37%	0.126%
58	16.874	2508	2514	2524	rBV2	40325	89218	8.89%	0.816%
59	17.045	2537	2543	2545	rBV5	12914	20864	2.08%	0.191%
60	17.309	2583	2588	2596	rVB2	20261	47026	4.68%	0.430%

Sum of corrected areas: 10931855

LSC Report - Integrated Chromatogram

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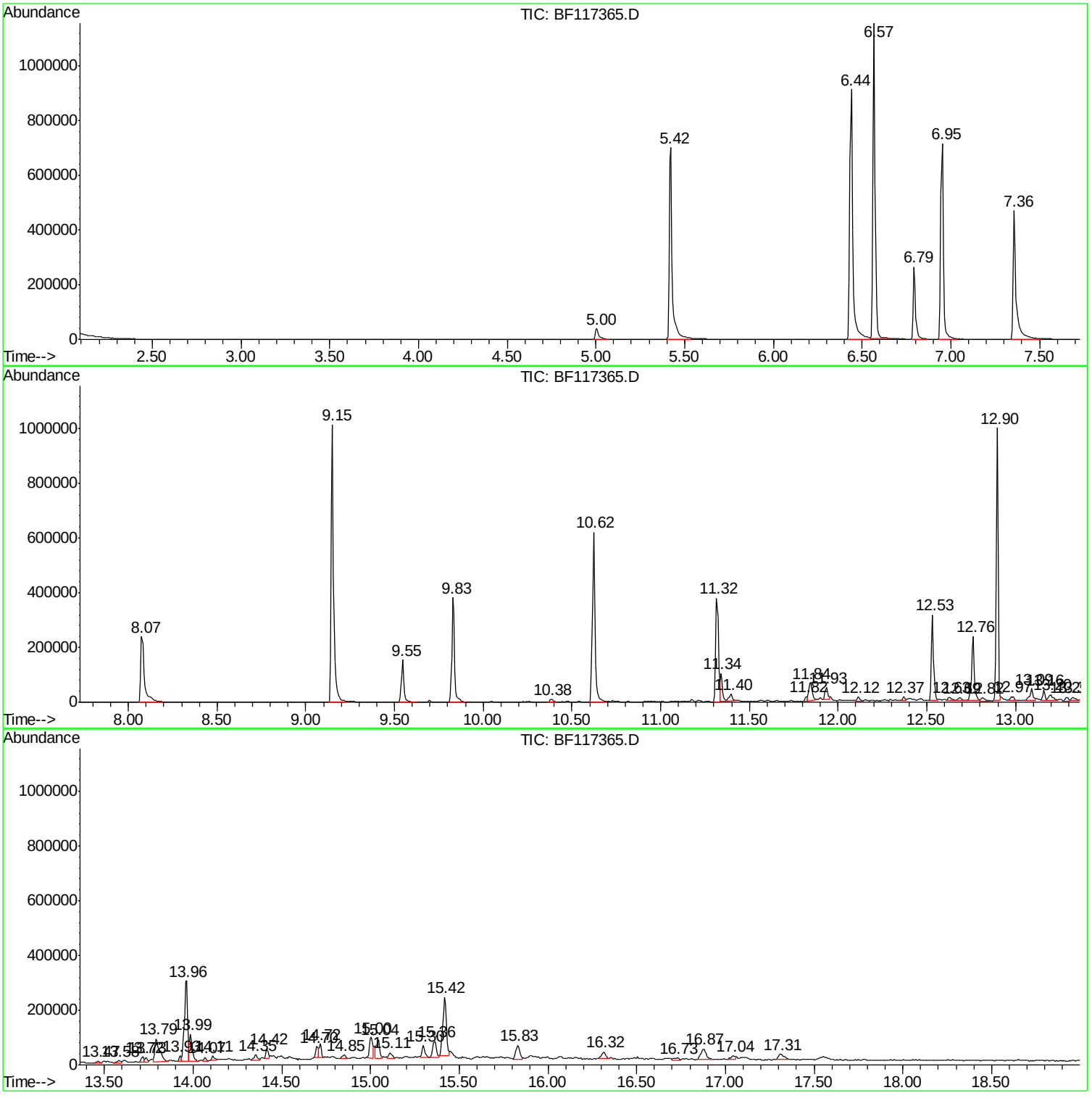
Operator : JU
Sample : K5297-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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\BF101019\
Data File : BF117365.D
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ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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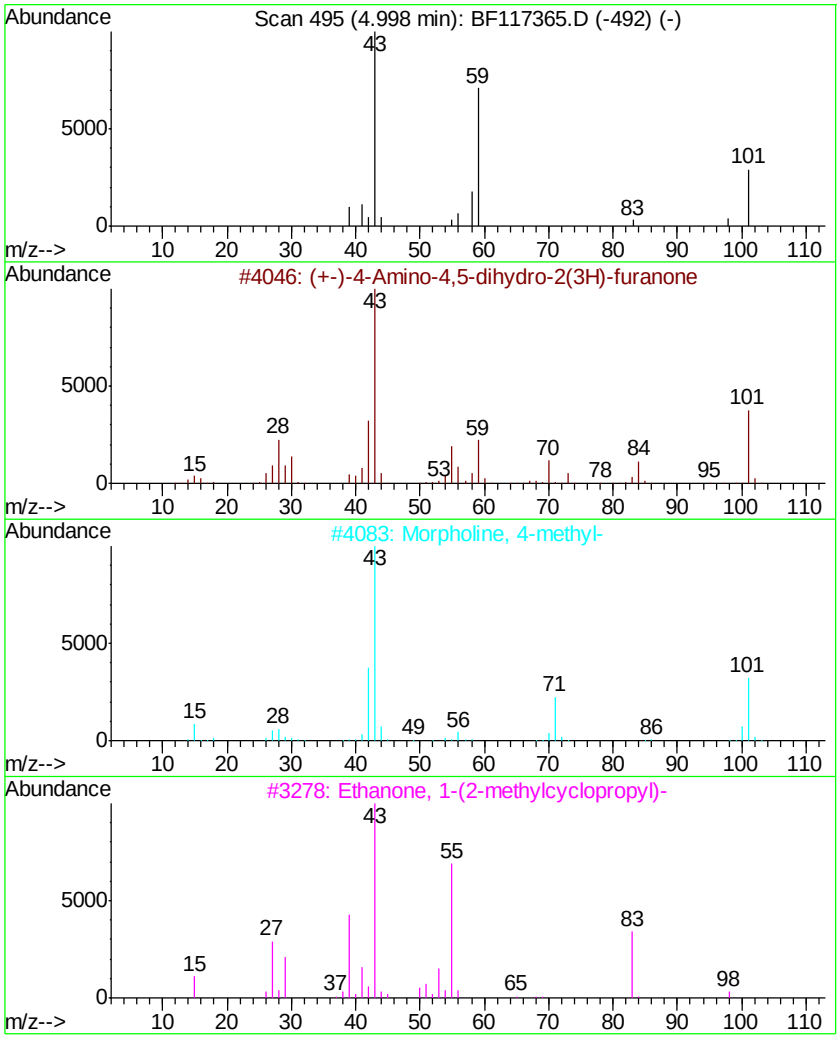
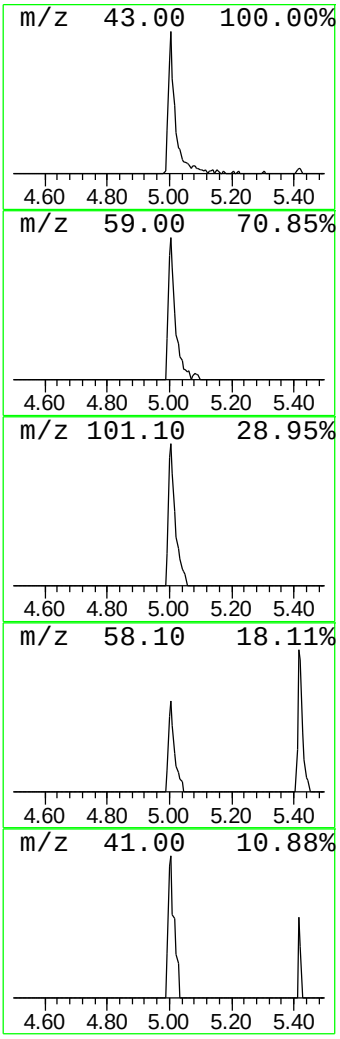
****

Peak Number 1 unknown5.00 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	4.81 ng	60204	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	28
2	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
3	Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101019\
Data File : BF117365.D
Acq On : 10 Oct 2019 17:35
Operator : JU
Sample : K5297-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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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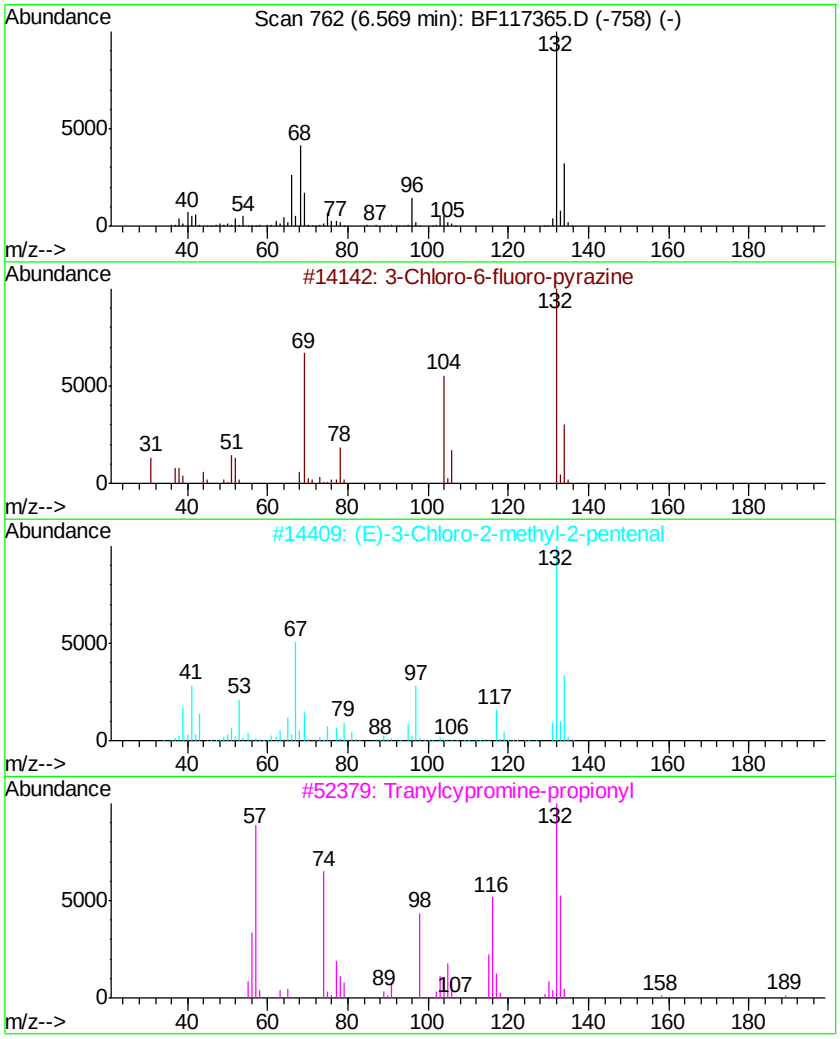
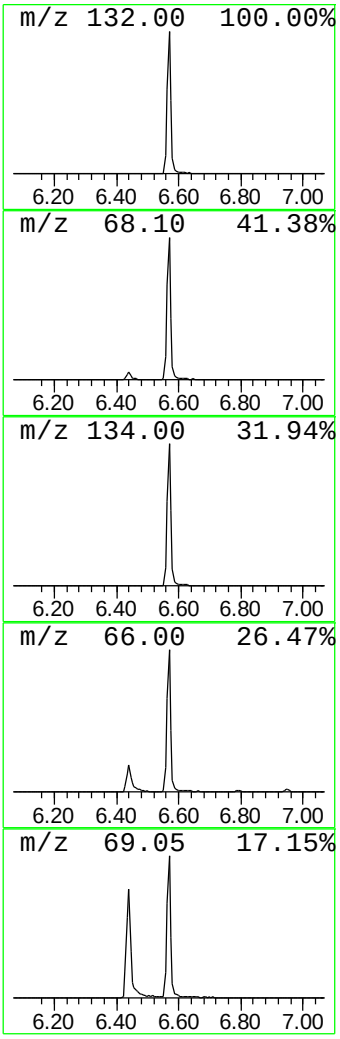
Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	80.21 ng	1003860	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101019\
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Acq On : 10 Oct 2019 17:35
Operator : JU
Sample : K5297-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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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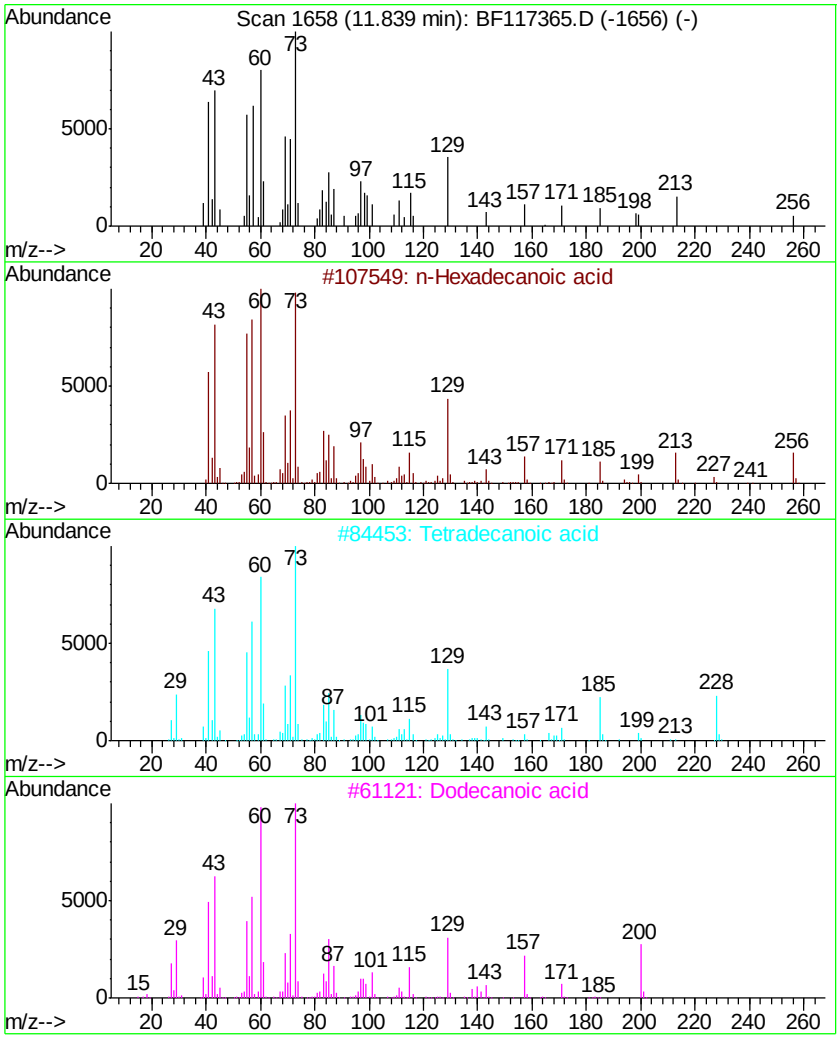
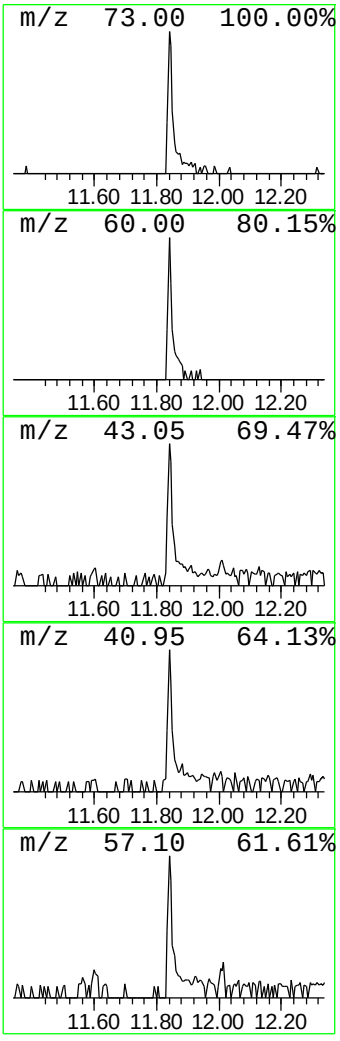
Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.84	4.48 ng	84172	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
3	Dodecanoic acid	200	C12H24O2	000143-07-7	72
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
5	n-Decanoic acid	172	C10H20O2	000334-48-5	59





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101019\
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Operator : JU
Sample : K5297-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

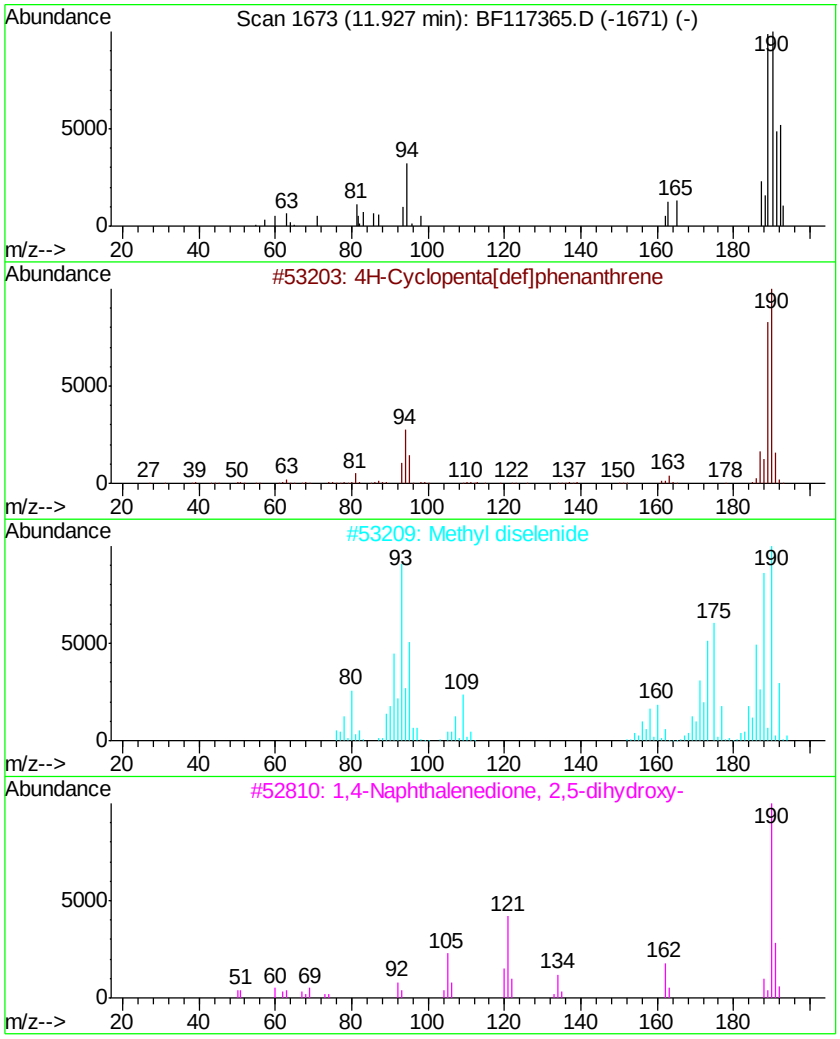
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

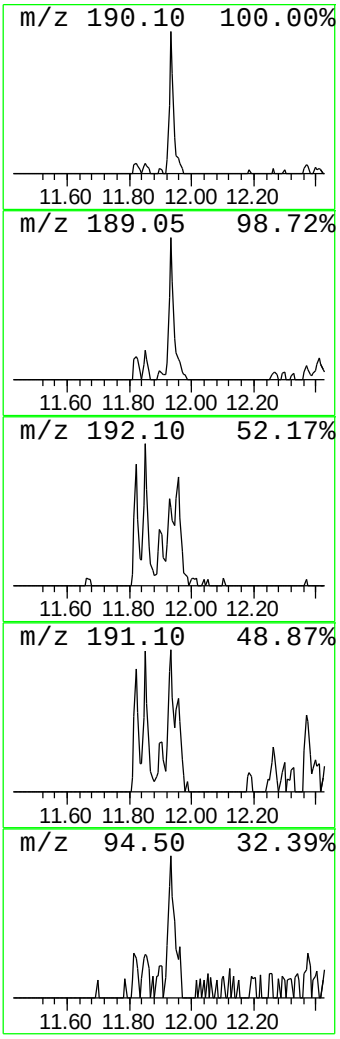
****

Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	2.41 ng	45232	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	83
2	Methyl diselenide	190	C2H6Se2	007101-31-7	55
3	1,4-Naphthalenedione, 2,5-dihydr...	190	C10H6O4	004923-55-1	17
4	5-Thiazolecarboxamide, 4-amino-2...	189	C5H7N3OS2	1000338-08-9	10
5	8H-Cyclopenta[d][1,2,4]triazolo[...	190	C9H10N4O	1000337-56-4	9





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Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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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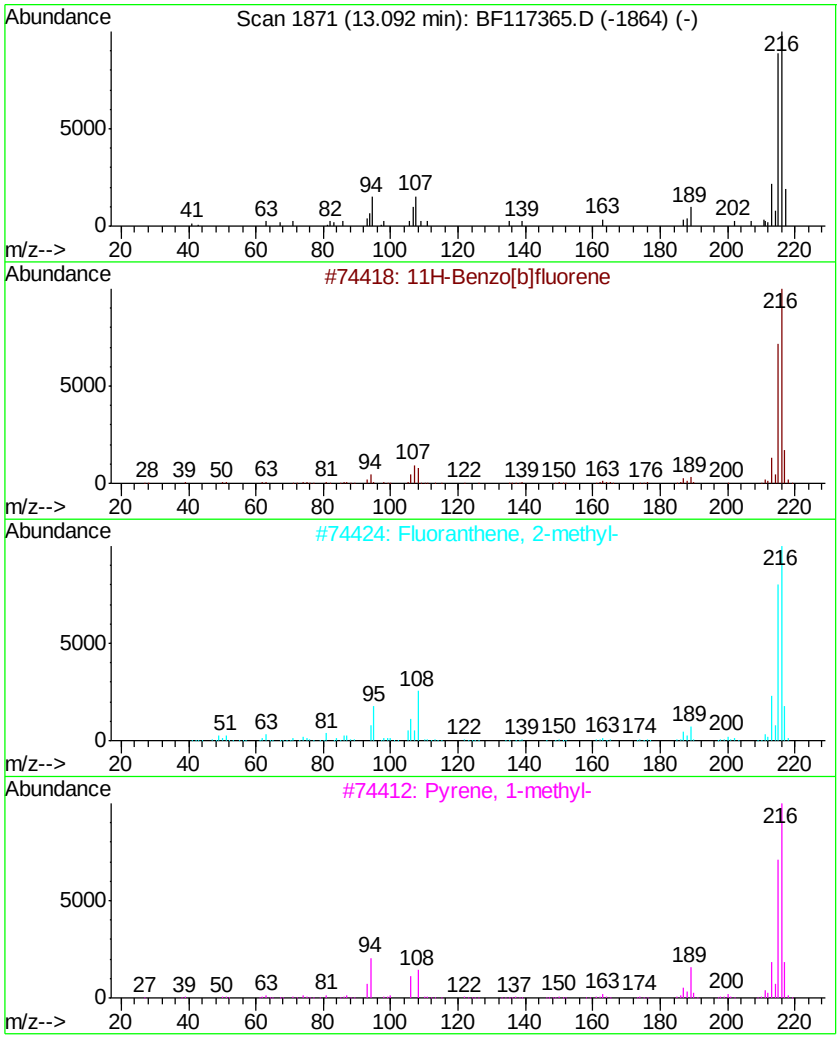
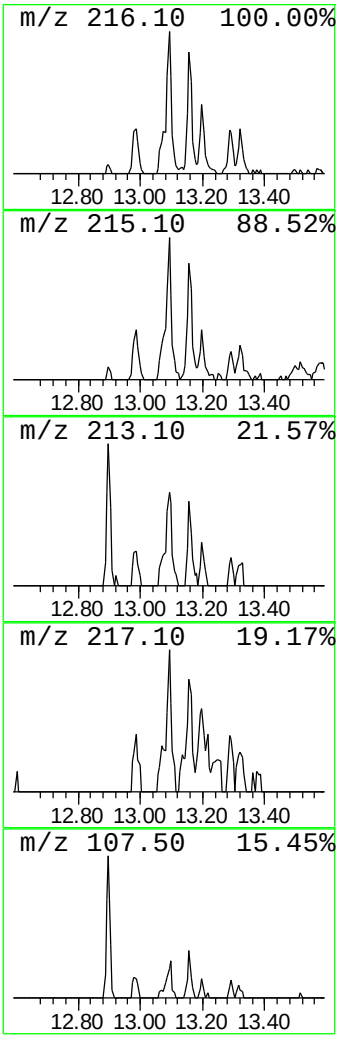
Peak Number 6 11H-Benzo[b]fluorene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.09	3.24 ng	60266	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	91
2	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	87
3	Pyrene, 1-methyl-	216	C17H12	002381-21-7	87
4	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	81
5	Pyrene, 2-methyl-	216	C17H12	003442-78-2	76





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ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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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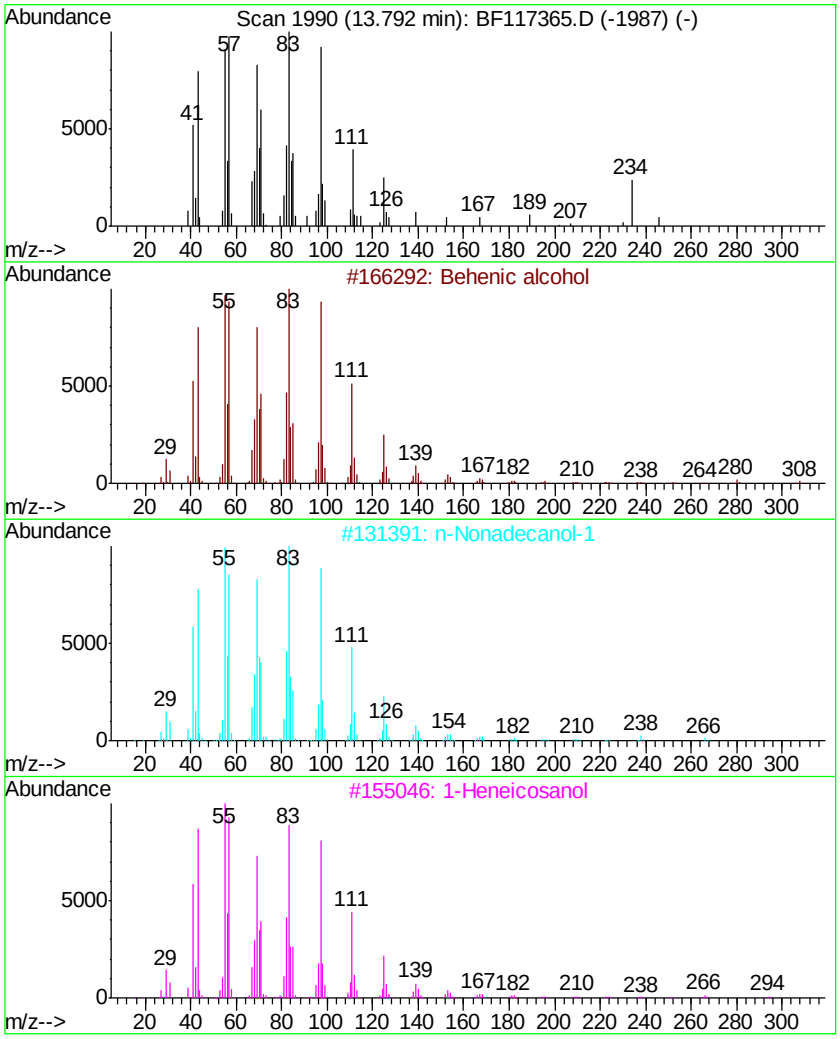
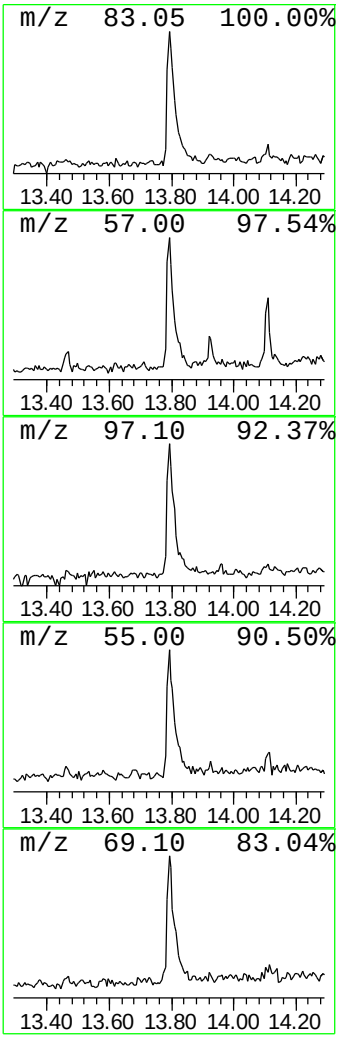
Peak Number 7 Behenic alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	8.37 ng	155740	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	91
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	91
3	1-Heneicosanol	312	C21H44O	015594-90-8	91
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	90
5	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	90





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Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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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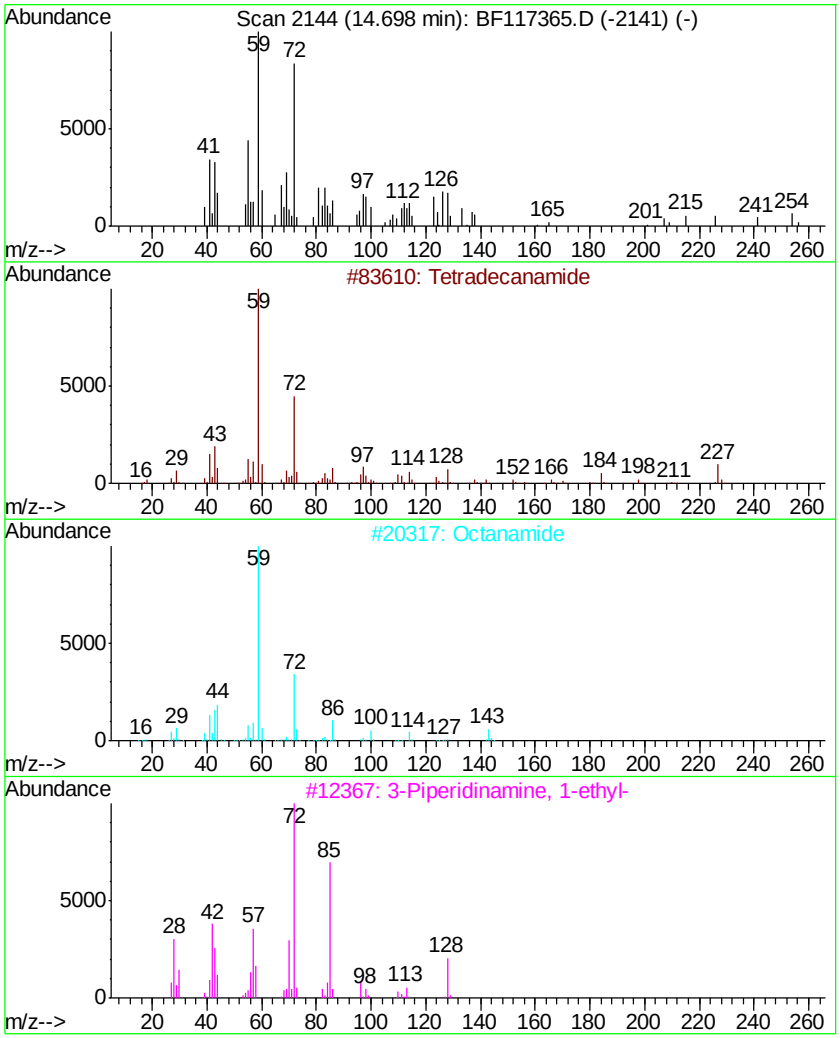
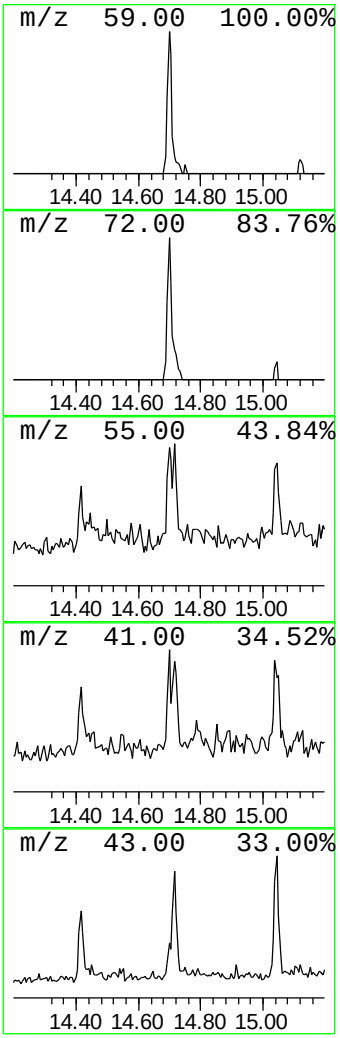
Peak Number 8 unknown14.70 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.70	2.33 ng	35339	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanamide	227	C14H29NO	000638-58-4	47
2	Octanamide	143	C8H17NO	000629-01-6	35
3	3-Piperidinamine, 1-ethyl-	128	C7H16N2	006789-94-2	30
4	5-Hydroxymethyl-2,2,5-trimethyl-...	256	C10H15F3O4	1000365-19-3	27
5	2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	27





Library Search Compound Report

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Data File : BF117365.D
Acq On : 10 Oct 2019 17:35
Operator : JU
Sample : K5297-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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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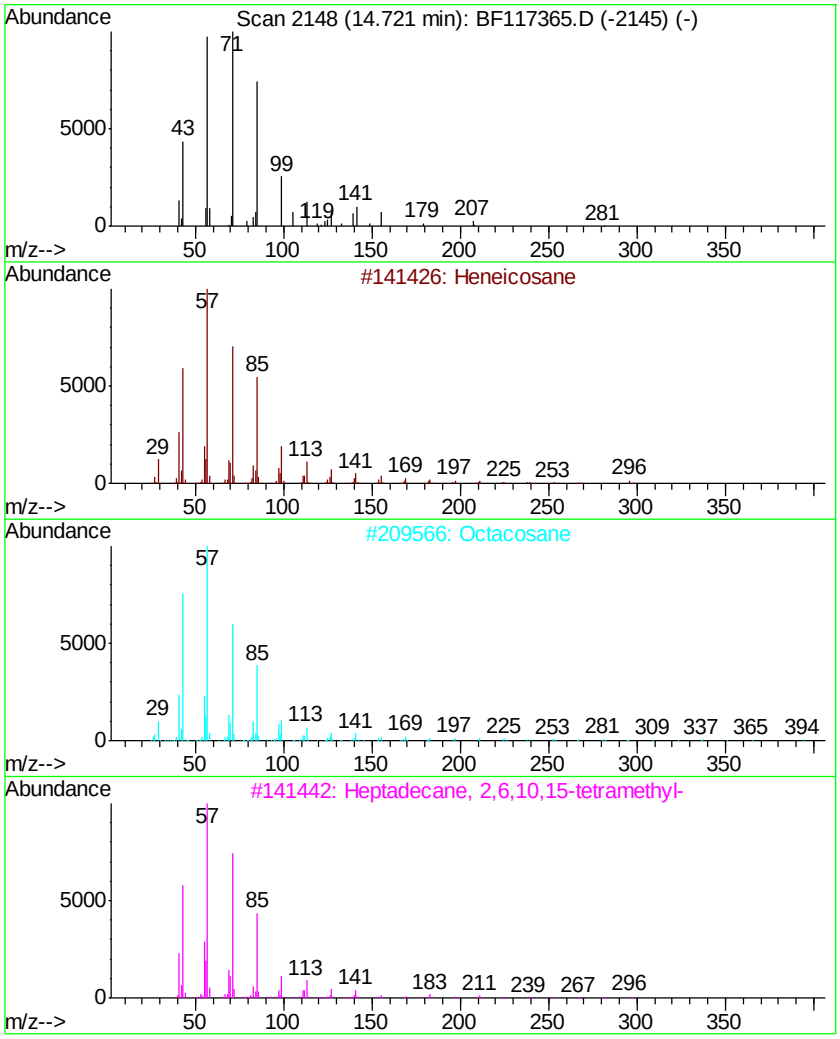
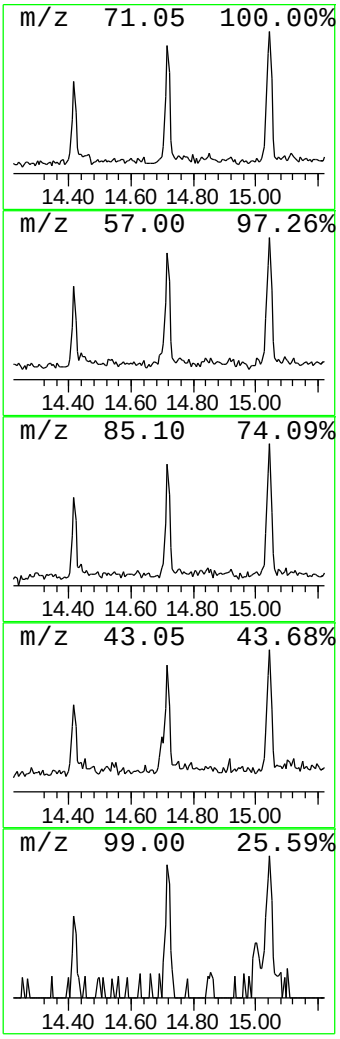
Peak Number 9 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	3.03 ng	46028	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	86
2	Octacosane	394	C28H58	000630-02-4	78
3	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	78
4	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	72
5	Nonane, 3-methyl-5-propyl-	184	C13H28	031081-18-2	64





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101019\
Data File : BF117365.D
Acq On : 10 Oct 2019 17:35
Operator : JU
Sample : K5297-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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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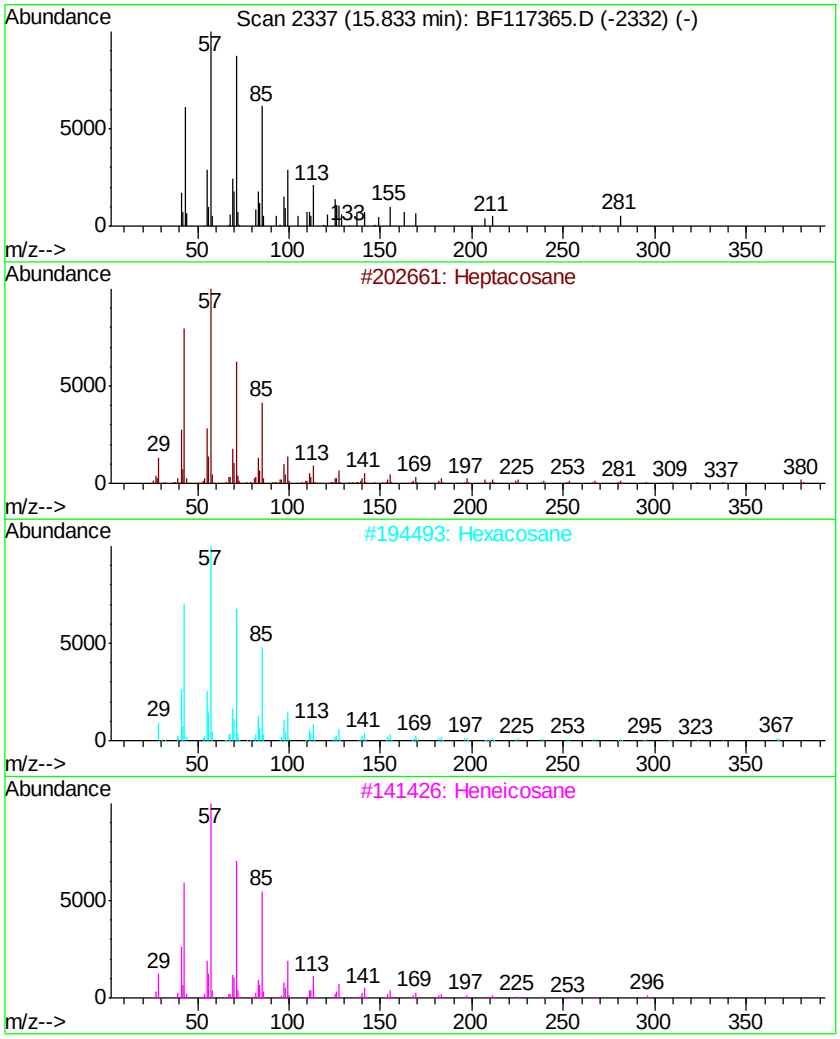
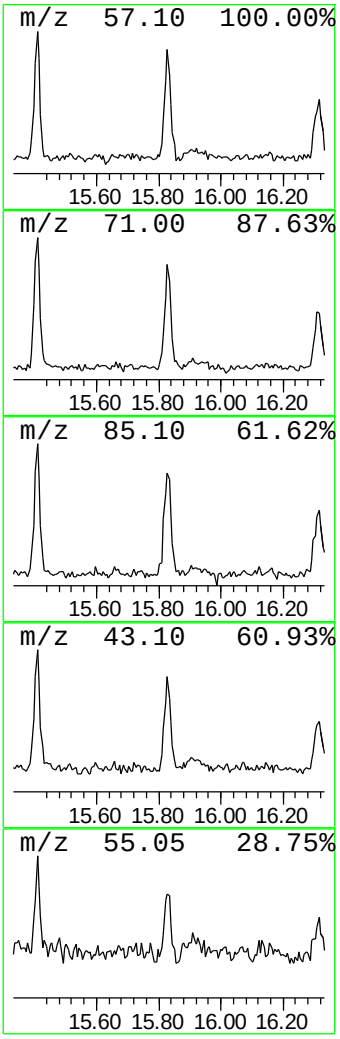
Peak Number 11 Heptacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.83	4.69 ng	71304	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Hexacosane	366	C26H54	000630-01-3	90
3	Heneicosane	296	C21H44	000629-94-7	90
4	Triacontane	422	C30H62	000638-68-6	87
5	Heptadecane	240	C17H36	000629-78-7	87





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101019\
Data File : BF117365.D
Acq On : 10 Oct 2019 17:35
Operator : JU
Sample : K5297-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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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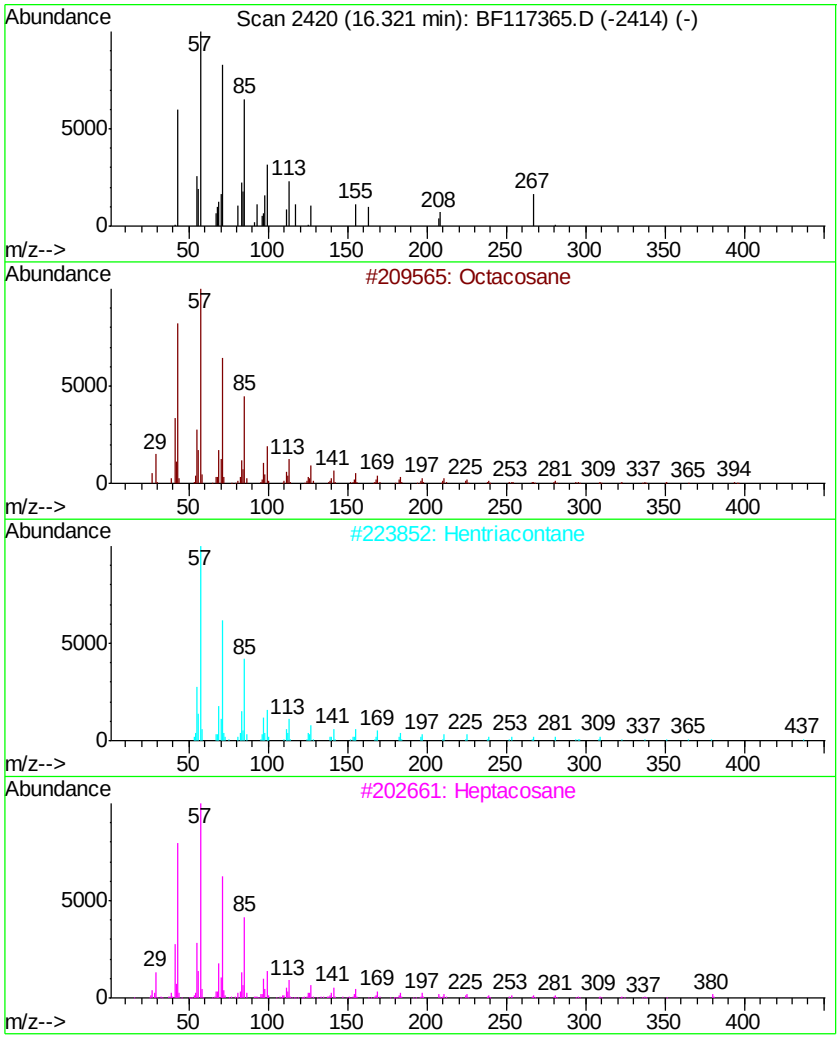
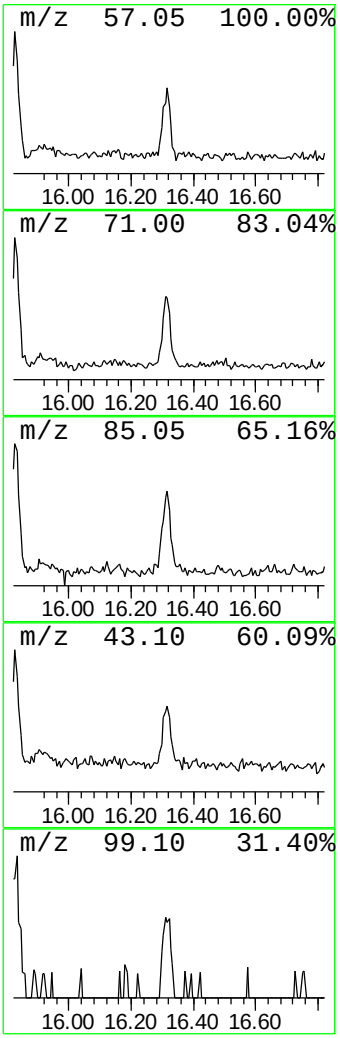
Peak Number 12 Octacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.32	2.71 ng	41228	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	80
2	Hentriacontane	437	C31H64	000630-04-6	72
3	Heptacosane	380	C27H56	000593-49-7	72
4	Hexadecane	226	C16H34	000544-76-3	72
5	Pentacosane	352	C25H52	000629-99-2	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101019\
Data File : BF117365.D
Acq On : 10 Oct 2019 17:35
Operator : JU
Sample : K5297-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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
unknown5.00	5.00	4.8	ng	60204	1	6.79	250317	20.0
unknown6.57	6.57	80.2	ng	1003860	1	6.79	250317	20.0
n-Hexadecanoic acid	11.84	4.5	ng	84172	4	11.32	375414	20.0
4H-Cyclopenta[def...	11.93	2.4	ng	45232	4	11.32	375414	20.0
11H-Benzo[b]fluorene	13.09	3.2	ng	60266	5	13.96	371974	20.0
Behenic alcohol	13.79	8.4	ng	155740	5	13.96	371974	20.0
unknown14.70	14.70	2.3	ng	35339	6	15.42	303940	20.0
Heneicosane	14.72	3.0	ng	46028	6	15.42	303940	20.0
Heptacosane	15.83	4.7	ng	71304	6	15.42	303940	20.0
Octacosane	16.32	2.7	ng	41228	6	15.42	303940	20.0