LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111919\
Data File : BF117862.D
Acq On : 19 Nov 2019 16:31
Operator : JU
Sample : K5865-16
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2-(2-4)

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-BF111319.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	2.199	13	19	25	rVB	690610	882503	19.27%	1.878%
2	5.128	512	517	529	rVB	575184	659804	14.41%	1.404%
3	5.528	580	585	588	rBV	3842712	3412332	74.52%	7.261%
4	6.534	751	756	773	rBV	3955354	3927437	85.77%	8.357%
5	6.681	777	781	784	rBV	4401704	3945708	86.17%	8.396%
6	6.916	817	821	824	rBV	1634927	1310409	28.62%	2.788%
7	7.069	843	847	851	rBV	3431890	3109553	67.91%	6.617%
8	7.475	911	916	919	rBV	2848727	2466489	53.86%	5.248%
9	8.204	1036	1040	1043	rBV	2010170	1728141	37.74%	3.677%
10	9.280	1219	1223	1226	rBV	5458226	4579215	100.00%	9.744%
11	9.675	1287	1290	1294	rVB	445144	362053	7.91%	0.770%
12	9.963	1335	1339	1343	rBV	2356179	1981411	43.27%	4.216%
13	10.751	1469	1473	1477	rBV	2672794	2460115	53.72%	5.235%
14	11.457	1589	1593	1595	rBV	2364639	1915885	41.84%	4.077%
15	11.480	1595	1597	1600	rVV	364369	283027	6.18%	0.602%
16	11.527	1600	1605	1608	rVB	128804	150796	3.29%	0.321%
17	11.957	1675	1678	1680	rBV	86117	92861	2.03%	0.198%
18	11.986	1680	1683	1686	rVB2	134242	145618	3.18%	0.310%
19	12.069	1694	1697	1700	rBV2	99700	121237	2.65%	0.258%
20	12.510	1769	1772	1775	rBV	67894	63640	1.39%	0.135%
21	12.592	1784	1786	1792	rVB	77061	76337	1.67%	0.162%
22	12.674	1796	1800	1803	rBV	1331156	1121970	24.50%	2.387%
23	12.768	1813	1816	1818	rBV	59479	62188	1.36%	0.132%
24	12.904	1833	1839	1842	rBV	1158516	1091065	23.83%	2.322%
25	13.045	1859	1863	1867	rVB	4377449	3844643	83.96%	8.181%
26	13.121	1871	1876	1880	rBV4	61328	111386	2.43%	0.237%
27	13.210	1888	1891	1892	rBV2	52717	63069	1.38%	0.134%
28	13.227	1892	1894	1898	rVB	89900	94735	2.07%	0.202%
29	13.333	1908	1912	1915	rBV	91351	85920	1.88%	0.183%
30	13.457	1931	1933	1937	rBV	50861	52249	1.14%	0.111%
31	13.621	1956	1961	1965	rBV5	34620	58249	1.27%	0.124%
32	13.739	1974	1981	1985	rBV	107191	127727	2.79%	0.272%
33	13.851	1995	2000	2003	rBV2	87541	113655	2.48%	0.242%
34	13.880	2003	2005	2007	rBV	66335	52449	1.15%	0.112%

LSC Area Percent Report

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Acq On : 19 Nov 2019 16:31
Operator : JU
Sample : K5865-16
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2-(2-4)

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-BF111319.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.945	2013	2016	2027	rBV5	99025	221610	4.84%	0.472%
36	14.104	2035	2043	2046	rBV2	1751312	2031406	44.36%	4.322%
37	14.127	2046	2047	2055	rVB	417018	293294	6.40%	0.624%
38	14.492	2106	2109	2112	rVB	69378	66735	1.46%	0.142%
39	14.574	2119	2123	2127	rBV4	122677	126452	2.76%	0.269%
40	14.892	2173	2177	2180	rBV	161143	164814	3.60%	0.351%
41	14.968	2187	2190	2194	rBV2	108182	131542	2.87%	0.280%
42	15.162	2218	2223	2226	rBV	299196	447265	9.77%	0.952%
43	15.245	2233	2237	2240	rBV	146802	169564	3.70%	0.361%
44	15.480	2273	2277	2283	rVB	149987	203528	4.44%	0.433%
45	15.539	2283	2287	2294	rVB	181846	245052	5.35%	0.521%
46	15.609	2294	2299	2303	rBV	1213471	1560348	34.07%	3.320%
47	15.645	2303	2305	2312	rVB2	200079	241454	5.27%	0.514%
48	16.104	2379	2383	2389	rVB2	107122	174295	3.81%	0.371%
49	16.639	2469	2474	2479	rBV3	52705	92433	2.02%	0.197%
50	17.133	2553	2558	2565	rVB2	72565	137601	3.00%	0.293%
51	17.598	2631	2637	2648	rVB	59378	134861	2.95%	0.287%

Sum of corrected areas: 46996130

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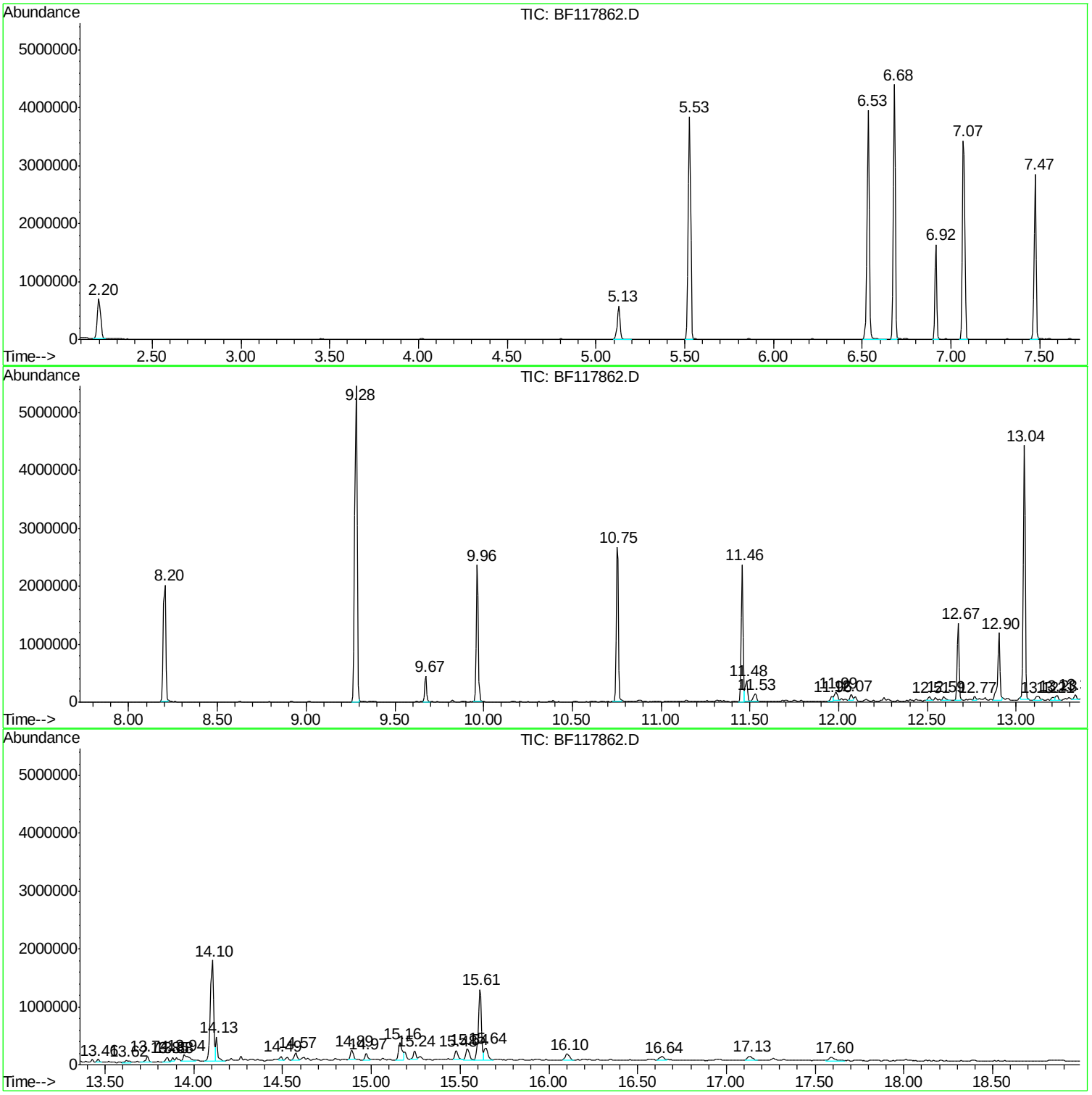
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
2-(2-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111919\
Data File : BF117862.D
Acq On : 19 Nov 2019 16:31
Operator : JU
Sample : K5865-16
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2-(2-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

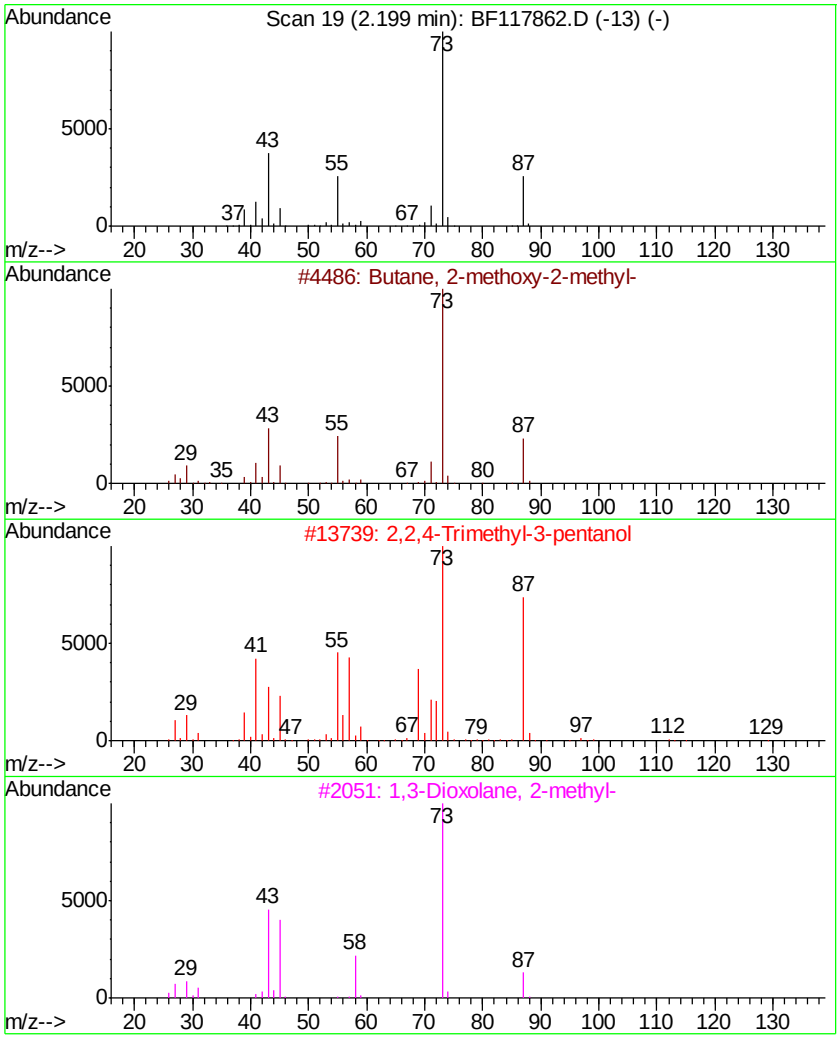
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

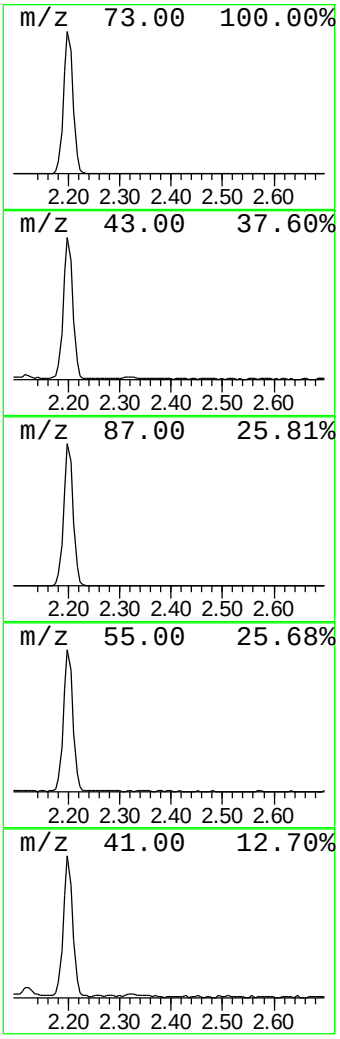
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.20	13.47 ng	882503	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111919\
Data File : BF117862.D
Acq On : 19 Nov 2019 16:31
Operator : JU
Sample : K5865-16
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2-(2-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

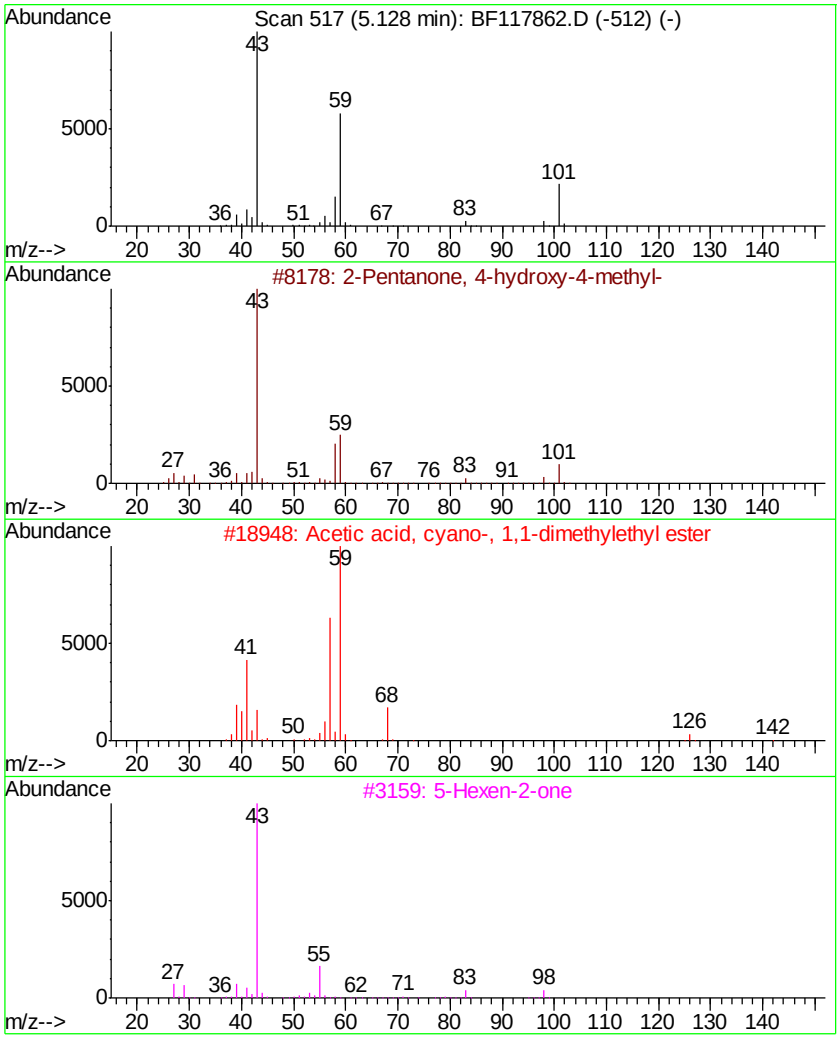
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

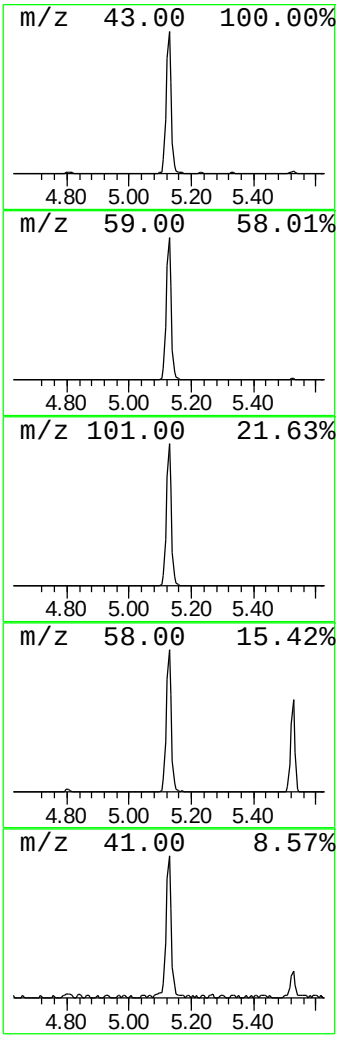
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	10.07 ng	659804	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111919\
Data File : BF117862.D
Acq On : 19 Nov 2019 16:31
Operator : JU
Sample : K5865-16
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2-(2-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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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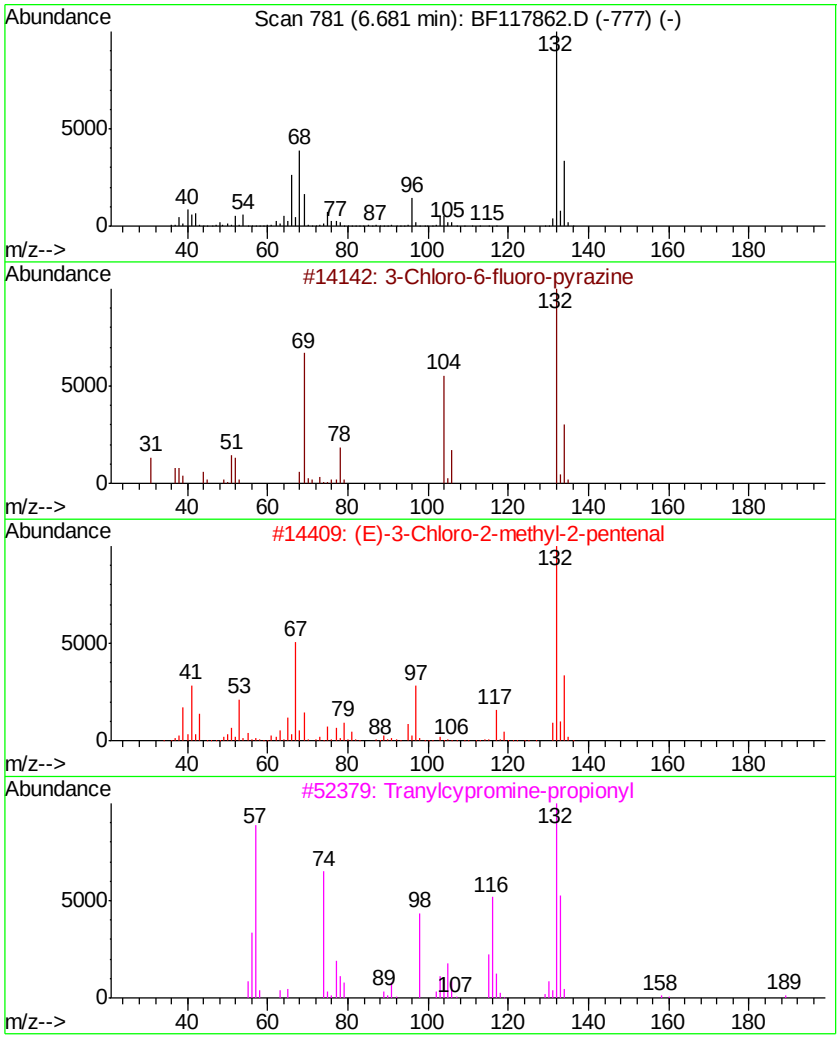
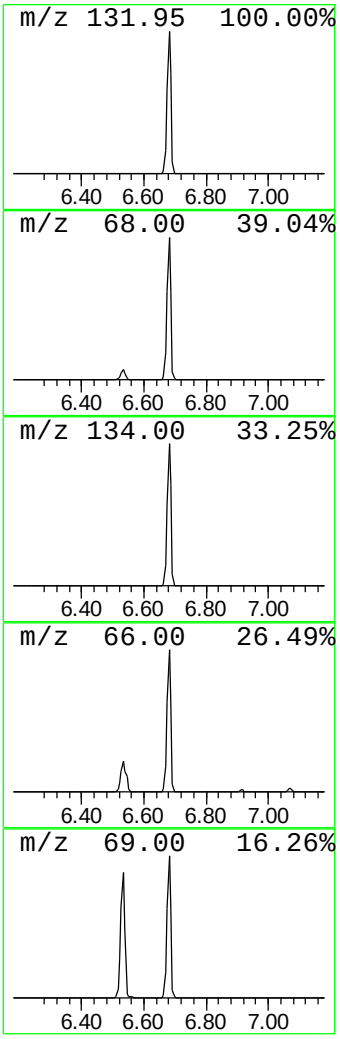
Peak Number 3 unknown6.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	60.22 ng	3945710	1,4-Dichlorobenzene-d4	6.92

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	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





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Instrument : BNA_F
ClientSampleId : 2-(2-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

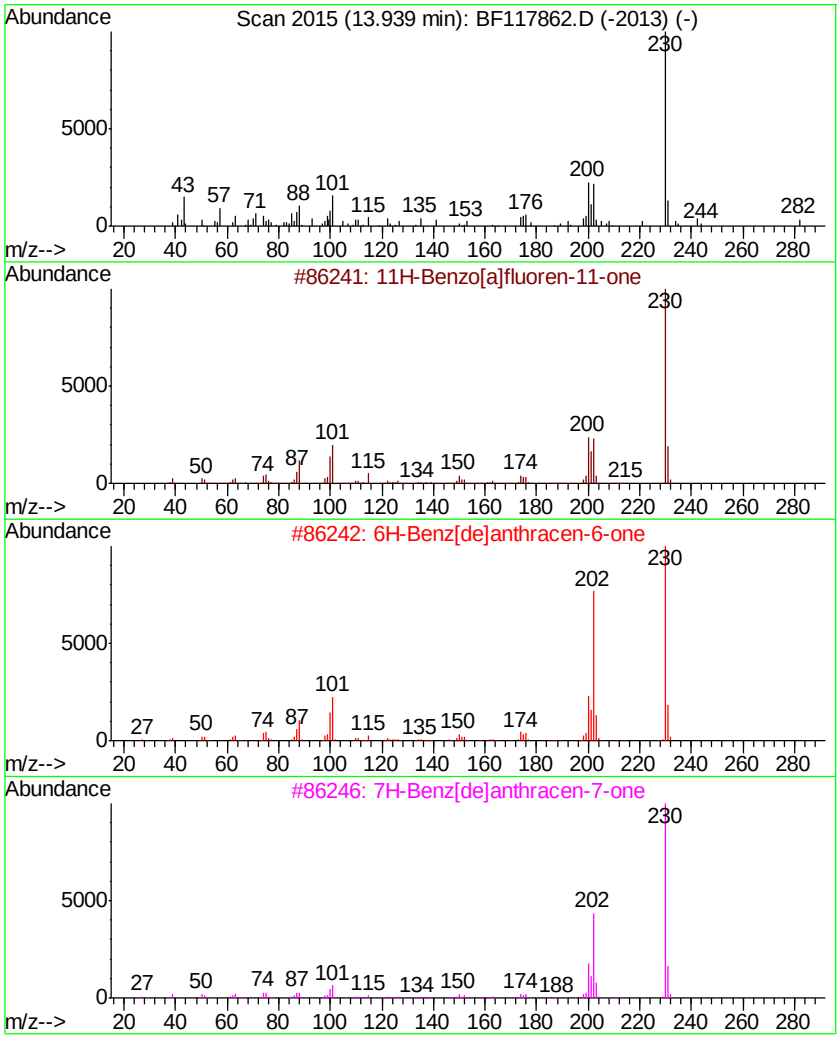
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

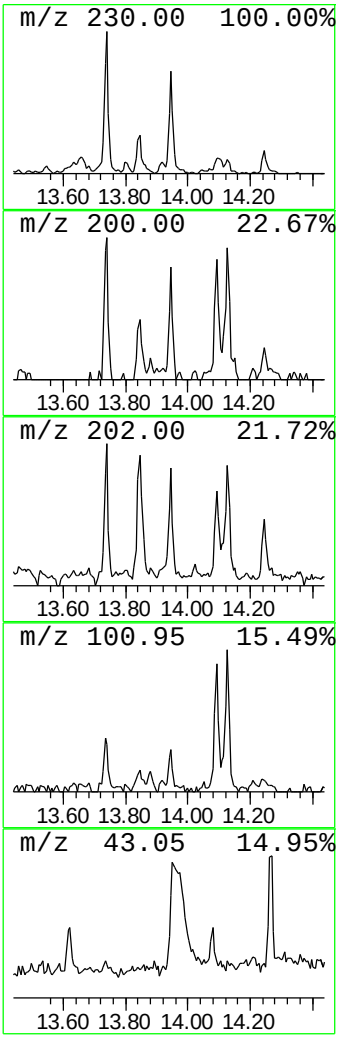
****

Peak Number 5 11H-Benzo[a]fluoren-11-one Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.94	2.18 ng	221610	Chrysene-d12	14.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	91
2	6H-Benz[de]anthracen-6-one	230	C17H10O	080252-14-8	86
3	7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	76
4	Dibenzo[c,h][2,6]naphthyridine	230	C16H10N2	000218-30-4	59
5	1-Pyrenecarboxaldehyde	230	C17H10O	003029-19-4	50





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Operator : JU
Sample : K5865-16
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2-(2-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

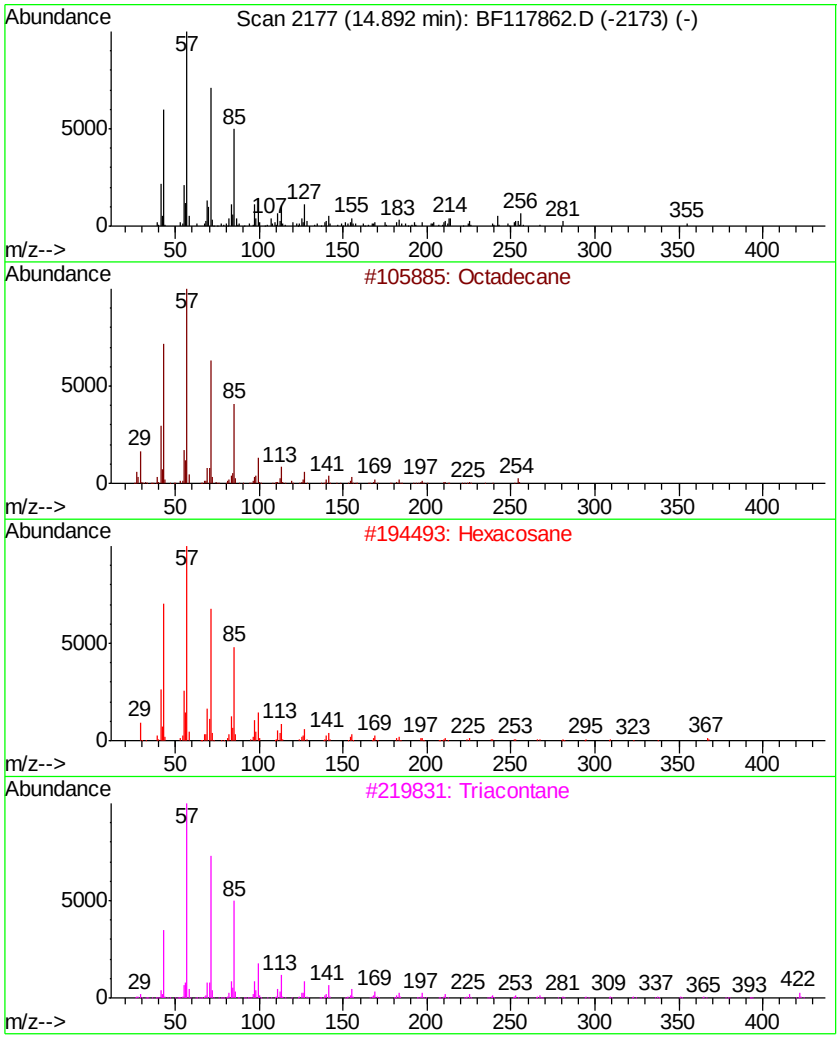
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

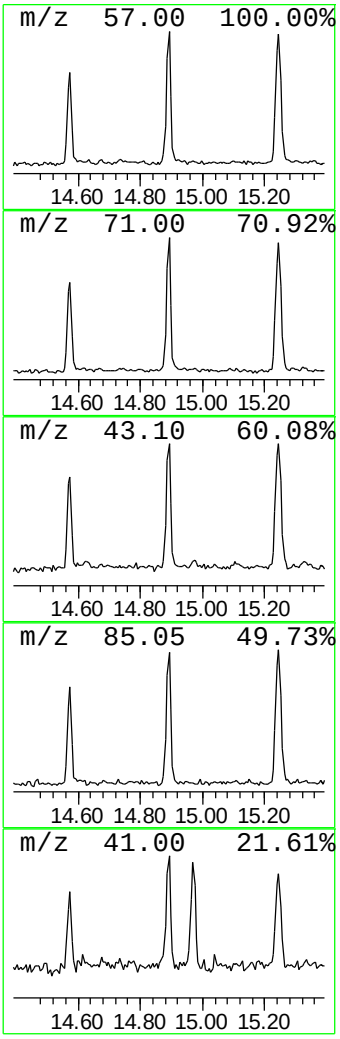
****

Peak Number 6 Octadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.89	2.11 ng	164814	Perylene-d12	15.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	98
2	Hexacosane	366	C26H54	000630-01-3	90
3	Triacontane	422	C30H62	000638-68-6	90
4	Hentriacontane	437	C31H64	000630-04-6	90
5	Heneicosane	296	C21H44	000629-94-7	90





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Acq On : 19 Nov 2019 16:31
Operator : JU
Sample : K5865-16
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2-(2-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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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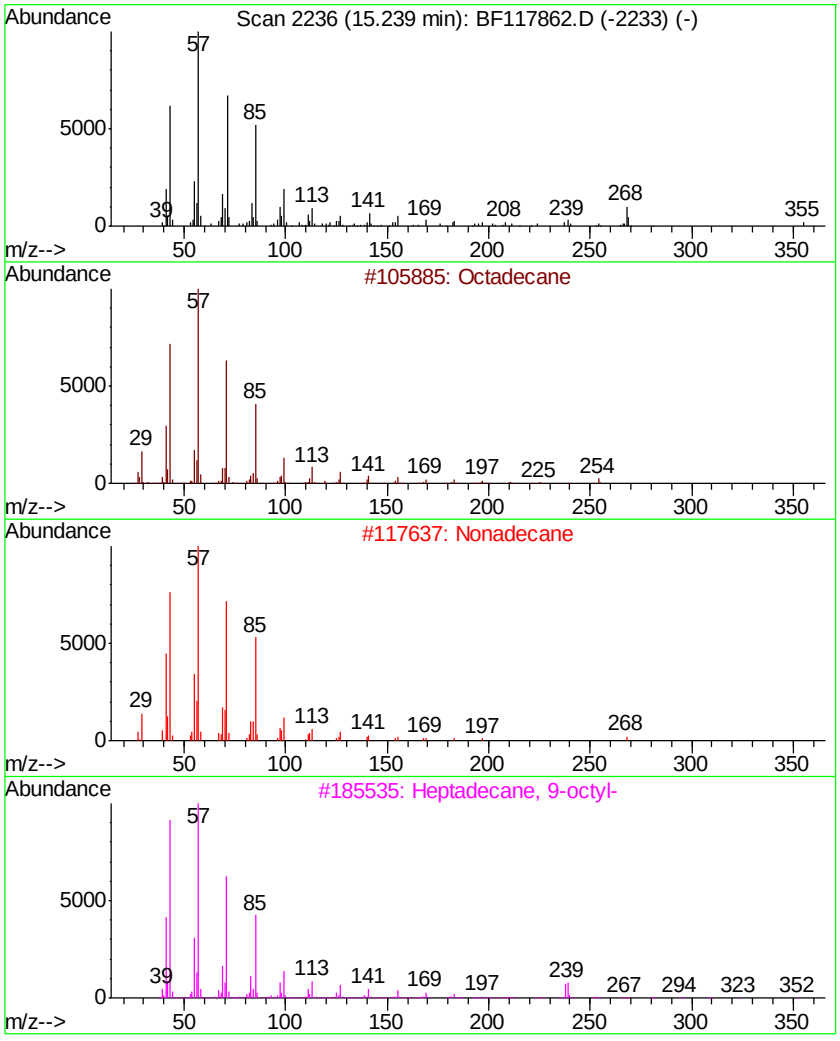
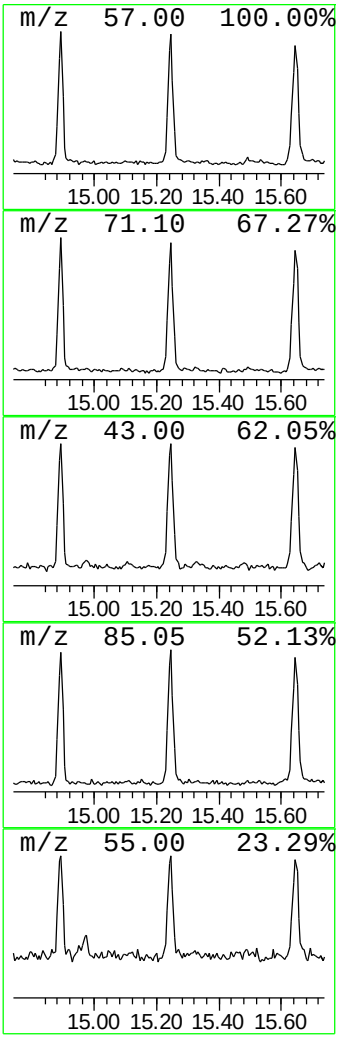
Peak Number 7 Nonadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.24	2.17 ng	169564	Perylene-d12	15.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	95
2	Nonadecane	268	C19H40	000629-92-5	90
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
4	Heptacosane	380	C27H56	000593-49-7	87
5	Hexacosane	366	C26H54	000630-01-3	87





Library Search Compound Report

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Data File : BF117862.D
Acq On : 19 Nov 2019 16:31
Operator : JU
Sample : K5865-16
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2-(2-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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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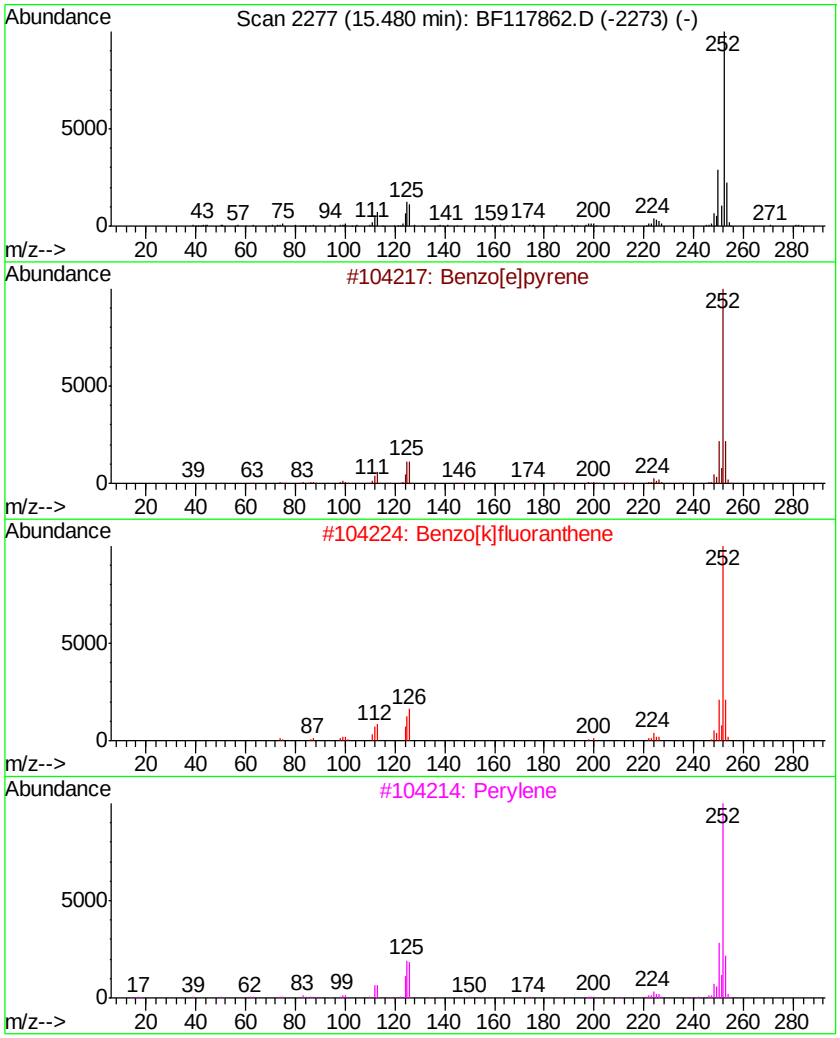
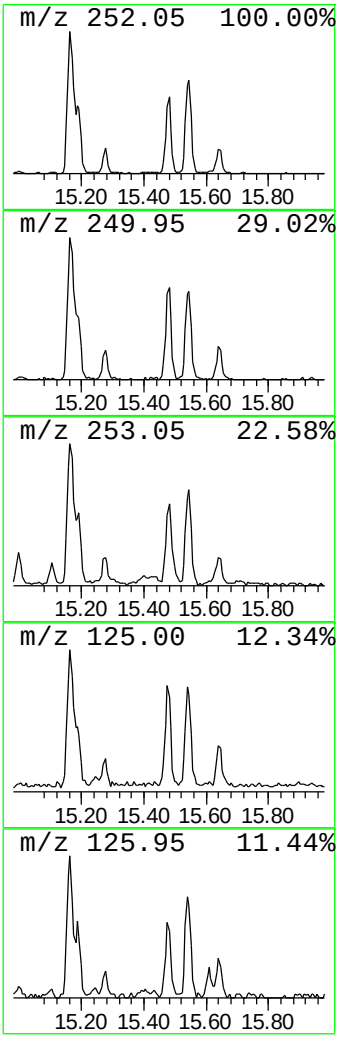
Peak Number 8 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.48	2.61 ng	203528	Perylene-d12	15.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
3	Perylene	252	C20H12	000198-55-0	96
4	Benzo[a]pyrene	252	C20H12	000050-32-8	95
5	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	94





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111919\
Data File : BF117862.D
Acq On : 19 Nov 2019 16:31
Operator : JU
Sample : K5865-16
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2-(2-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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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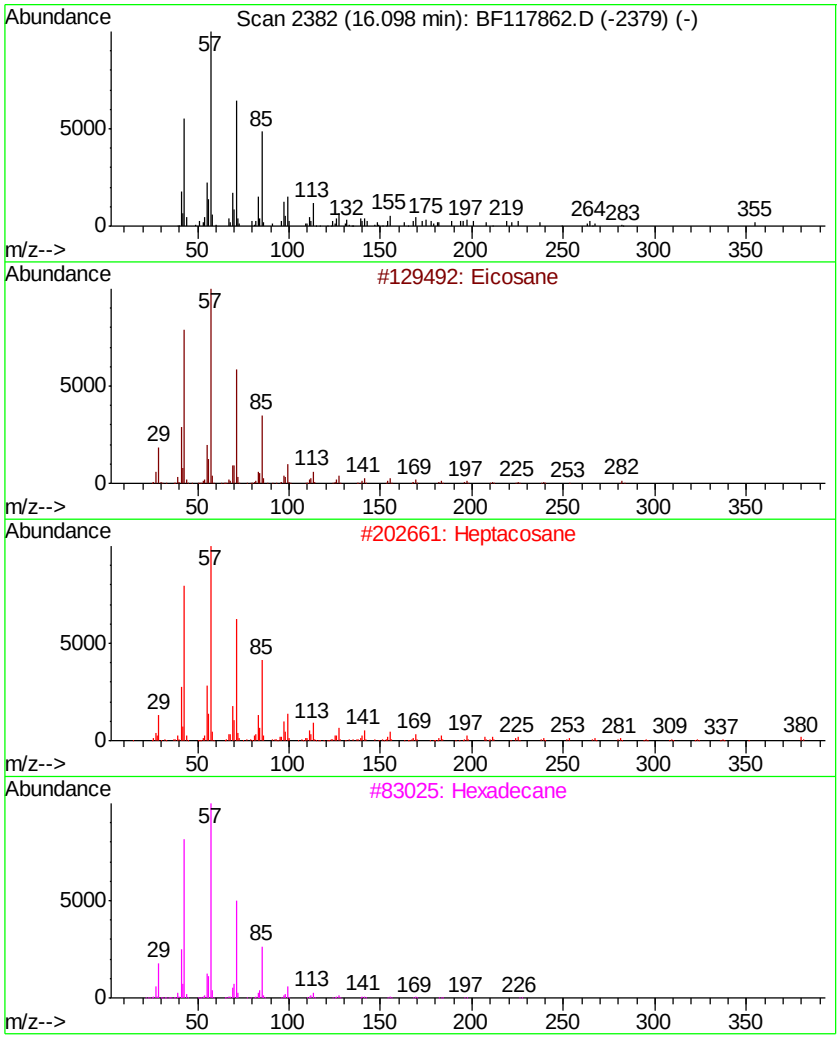
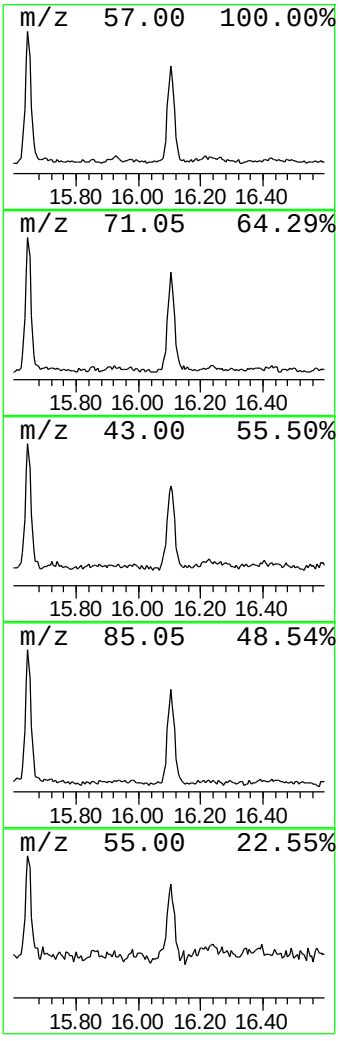
Peak Number 9 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.10	2.23 ng	174295	Perylene-d12	15.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	94
2	Heptacosane	380	C27H56	000593-49-7	91
3	Hexadecane	226	C16H34	000544-76-3	90
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
5	Heneicosane	296	C21H44	000629-94-7	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF111919\
Data File : BF117862.D
Acq On : 19 Nov 2019 16:31
Operator : JU
Sample : K5865-16
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2-(2-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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
Butane, 2-methoxy...	2.20	13.5	ng	882503	1	6.92	1310410	20.0
2-Pentanone, 4-hy...	5.13	10.1	ng	659804	1	6.92	1310410	20.0
unknown6.68	6.68	60.2	ng	3945710	1	6.92	1310410	20.0
11H-Benzo[a]fluor...	13.94	2.2	ng	221610	5	14.10	2031410	20.0
Octadecane	14.89	2.1	ng	164814	6	15.61	1560350	20.0
Nonadecane	15.24	2.2	ng	169564	6	15.61	1560350	20.0
Benzo[e]pyrene	15.48	2.6	ng	203528	6	15.61	1560350	20.0
Eicosane	16.10	2.2	ng	174295	6	15.61	1560350	20.0