LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010919\
Data File : BF111941.D
Acq On : 9 Jan 2019 10:45
Operator : JU/SJ
Sample : K1066-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TN-1419

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-BF010719.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	2.251	24	28	45	rVB	129897	217415	4.23%	0.445%
2	3.481	234	237	250	rBV	27116	63415	1.23%	0.130%
3	5.122	511	516	522	rBV	197821	249775	4.86%	0.511%
4	5.204	526	530	542	rVB	455301	443352	8.63%	0.907%
5	5.528	580	585	588	rBV	4131775	3820296	74.37%	7.815%
6	6.528	750	755	762	rBV	4006034	4252842	82.78%	8.700%
7	6.663	773	778	781	rBV	4436760	4167880	81.13%	8.527%
8	6.886	812	816	819	rBV	1276163	1179517	22.96%	2.413%
9	7.045	838	843	846	rBV	3312240	3284906	63.94%	6.720%
10	7.445	905	911	914	rBV	2668250	2727735	53.10%	5.580%
11	8.169	1028	1034	1037	rBV	1770812	1727639	33.63%	3.534%
12	8.880	1150	1155	1161	rVB	76521	63690	1.24%	0.130%
13	9.245	1211	1217	1220	rBV	5078687	5137218	100.00%	10.510%
14	9.627	1279	1282	1287	rVB	424306	400733	7.80%	0.820%
15	9.922	1325	1332	1336	rBV	2130897	2103091	40.94%	4.302%
16	10.469	1422	1425	1431	rVB2	54264	60894	1.19%	0.125%
17	10.716	1461	1467	1470	rBV	3801435	3572087	69.53%	7.308%
18	10.810	1480	1483	1486	rBV	49771	67964	1.32%	0.139%
19	10.839	1486	1488	1495	rVB	66481	62453	1.22%	0.128%
20	11.274	1556	1562	1565	rBV3	40708	63151	1.23%	0.129%
21	11.410	1580	1585	1588	rBV	2387944	2214748	43.11%	4.531%
22	11.433	1588	1589	1593	rVV	456618	270441	5.26%	0.553%
23	11.486	1595	1598	1600	rVB	69549	62506	1.22%	0.128%
24	11.639	1618	1624	1632	rBV2	38426	64610	1.26%	0.132%
25	11.933	1672	1674	1681	rVB3	285555	261786	5.10%	0.536%
26	12.021	1686	1689	1692	rBV	86164	96726	1.88%	0.198%
27	12.621	1788	1791	1796	rVB	672381	589860	11.48%	1.207%
28	12.851	1825	1830	1835	rBV	477495	556380	10.83%	1.138%
29	12.998	1847	1855	1858	rBV	5231434	4916469	95.70%	10.058%
30	13.180	1883	1886	1888	rVB	80112	72195	1.41%	0.148%
31	13.221	1888	1893	1895	rBV	61919	58543	1.14%	0.120%
32	13.286	1900	1904	1906	rBV2	59062	56918	1.11%	0.116%
33	13.468	1928	1935	1941	rVB6	48291	87032	1.69%	0.178%
34	13.563	1946	1951	1954	rBV2	87903	103077	2.01%	0.211%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010919\
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Operator : JU/SJ
Sample : K1066-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TN-1419

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-BF010719.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.686	1965	1972	1977	rBV	54922	88905	1.73%	0.182%
36	13.798	1985	1991	1994	rBV2	59691	90708	1.77%	0.186%
37	13.892	2003	2007	2014	rVB2	235002	268472	5.23%	0.549%
38	14.051	2026	2034	2037	rBV	1789230	1948888	37.94%	3.987%
39	14.074	2037	2038	2045	rVB	247307	217680	4.24%	0.445%
40	14.210	2058	2061	2065	rBV	127621	114460	2.23%	0.234%
41	14.515	2110	2113	2119	rVB2	179247	185740	3.62%	0.380%
42	14.827	2163	2166	2170	rVB	168942	169448	3.30%	0.347%
43	14.904	2176	2179	2183	rBV2	42873	51637	1.01%	0.106%
44	15.098	2208	2212	2215	rBV	165309	241472	4.70%	0.494%
45	15.168	2221	2224	2228	rVB	142365	151165	2.94%	0.309%
46	15.404	2261	2264	2269	rVB	98565	132368	2.58%	0.271%
47	15.468	2271	2275	2280	rVV	133910	182090	3.54%	0.373%
48	15.539	2281	2287	2300	rVB	996584	1462758	28.47%	2.992%
49	16.004	2361	2366	2373	rBV2	104349	173014	3.37%	0.354%
50	16.515	2449	2453	2460	rVB	76532	127987	2.49%	0.262%
51	17.027	2536	2540	2548	rVB2	65211	126820	2.47%	0.259%
52	17.474	2613	2616	2621	rVB2	43865	70263	1.37%	0.144%

Sum of corrected areas: 48881219

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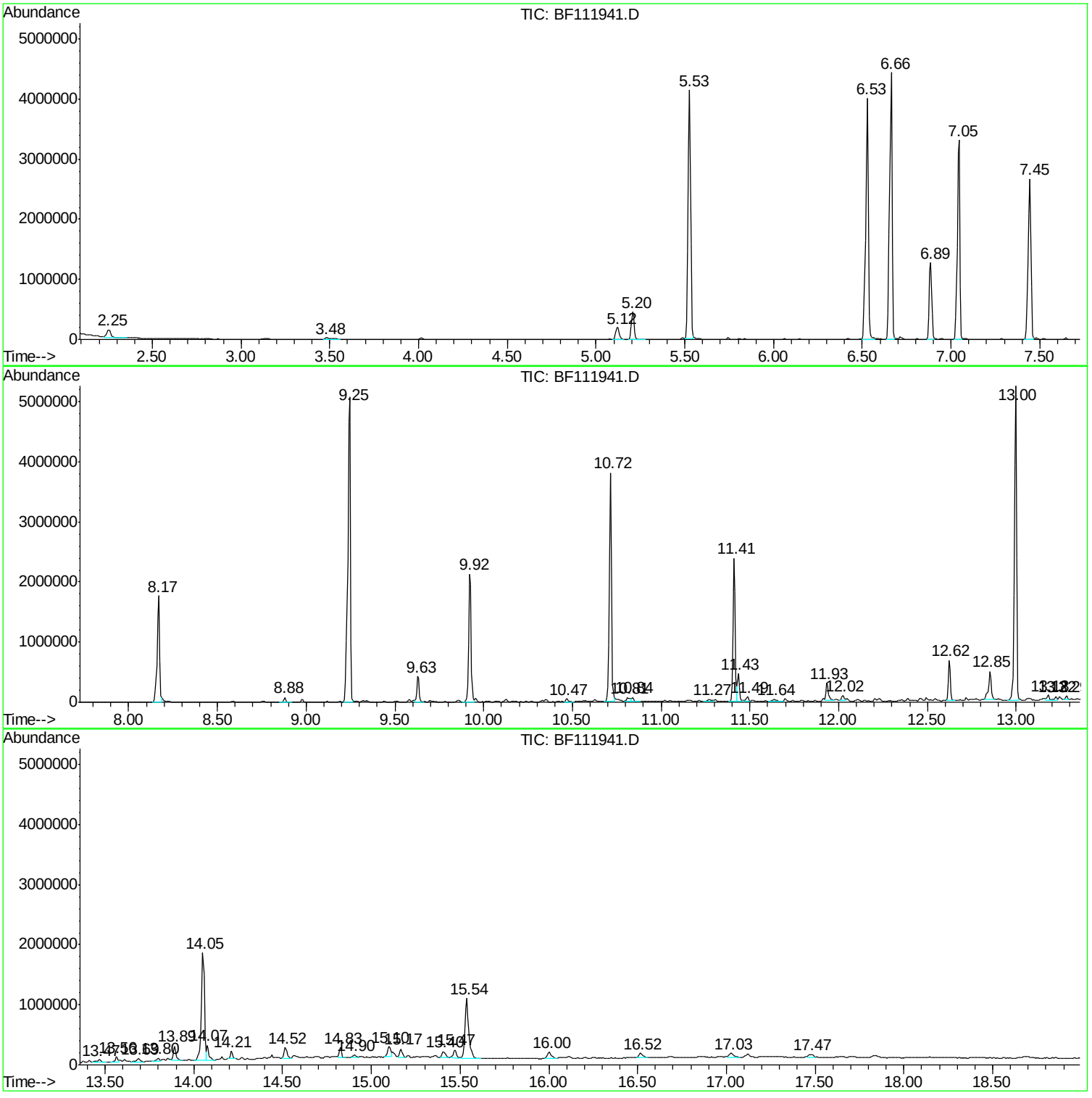
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TN-1419

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.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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Operator : JU/SJ
Sample : K1066-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TN-1419

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

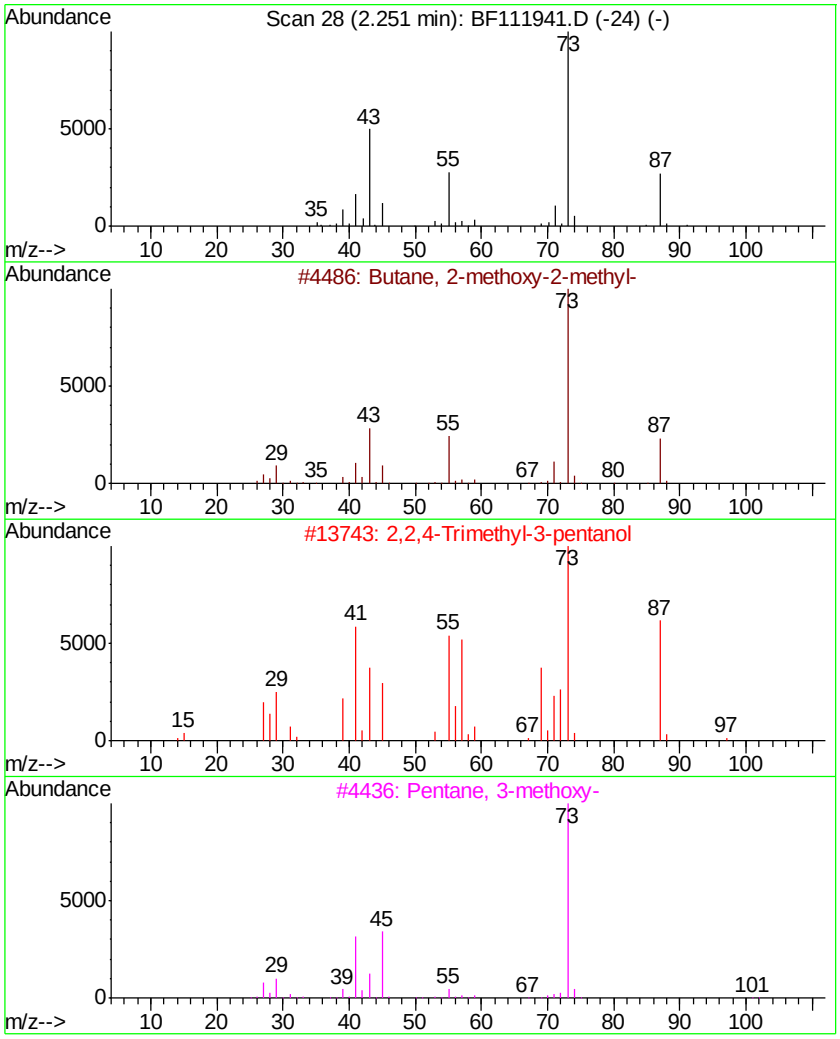
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

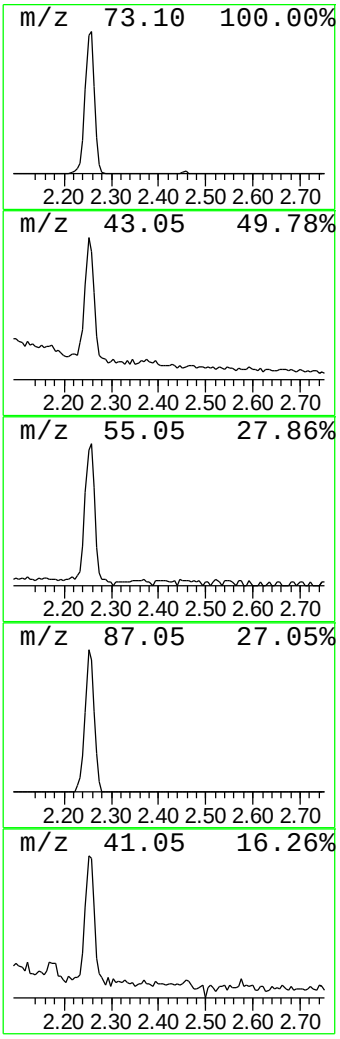
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.25	3.69 ng	217415	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	43
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





Library Search Compound Report

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Operator : JU/SJ
Sample : K1066-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TN-1419

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.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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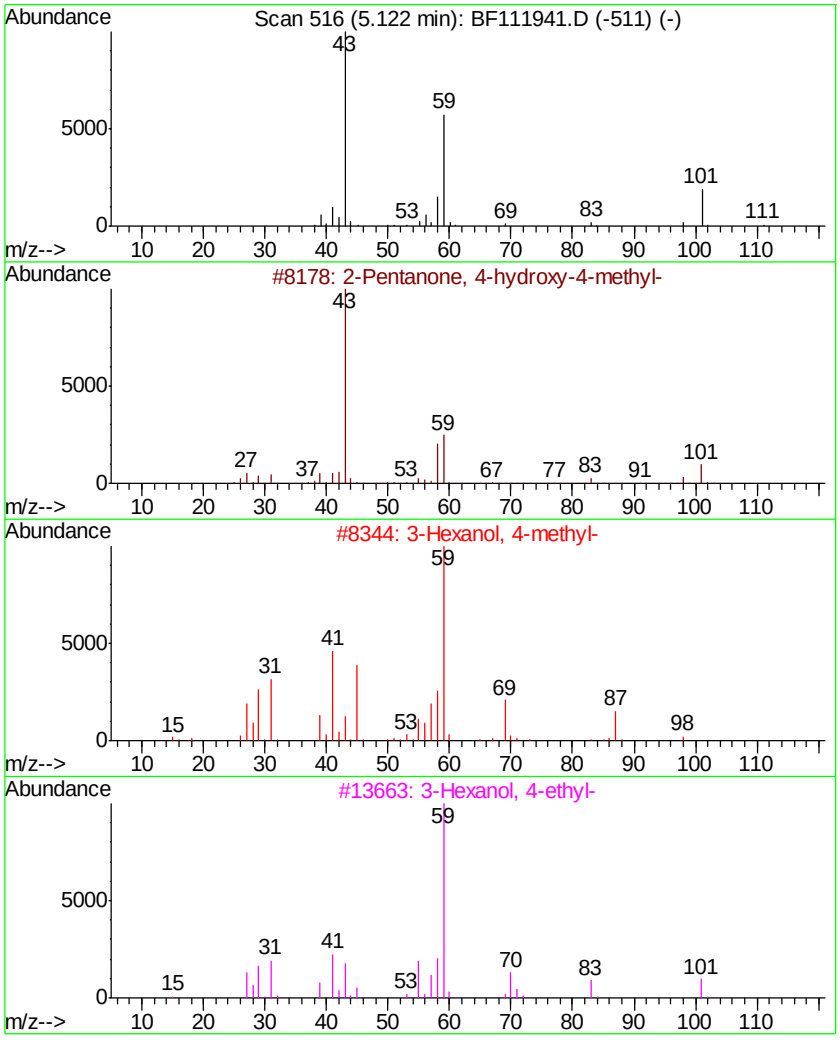
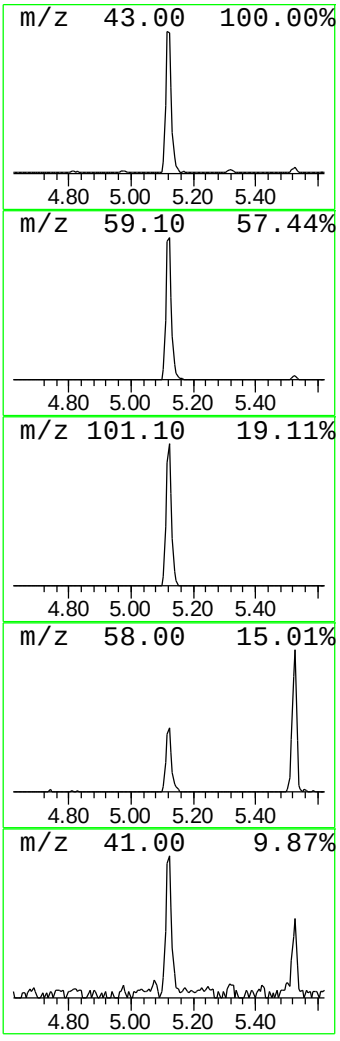
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	4.24 ng	249775	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3	3-Hexanol, 4-ethyl-	130	C8H18O	019780-44-0	28
4	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17
5	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010919\
Data File : BF111941.D
Acq On : 9 Jan 2019 10:45
Operator : JU/SJ
Sample : K1066-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TN-1419

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

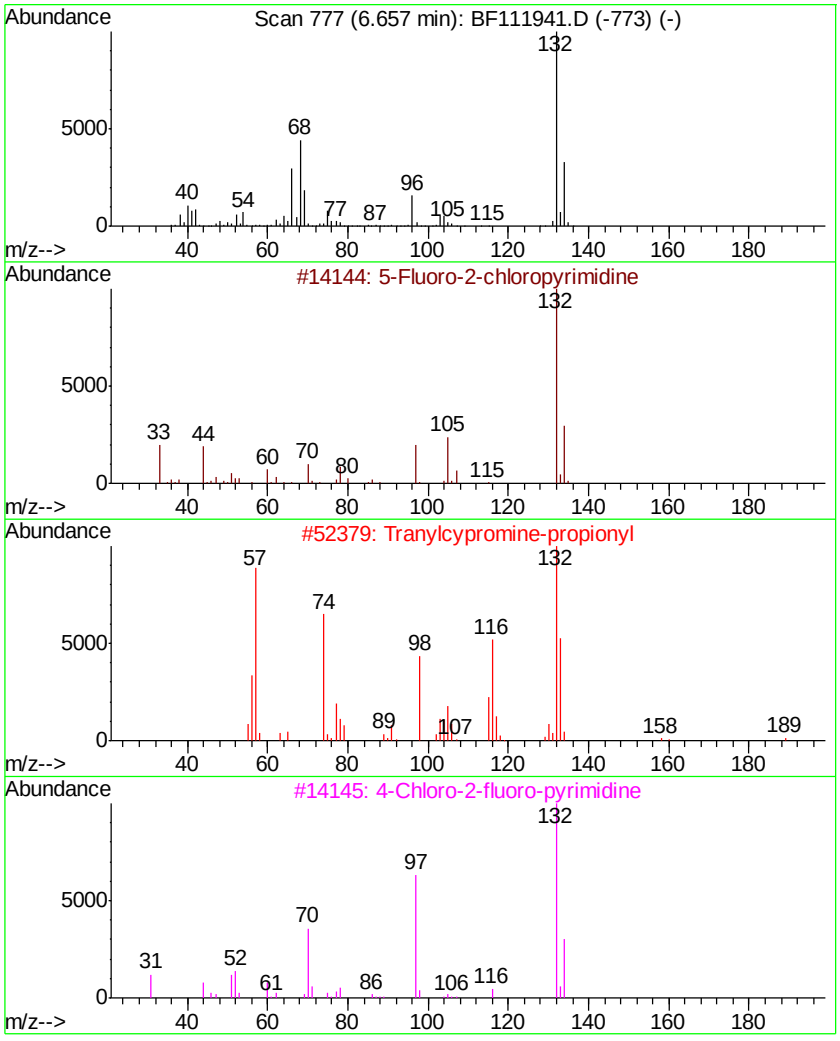
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

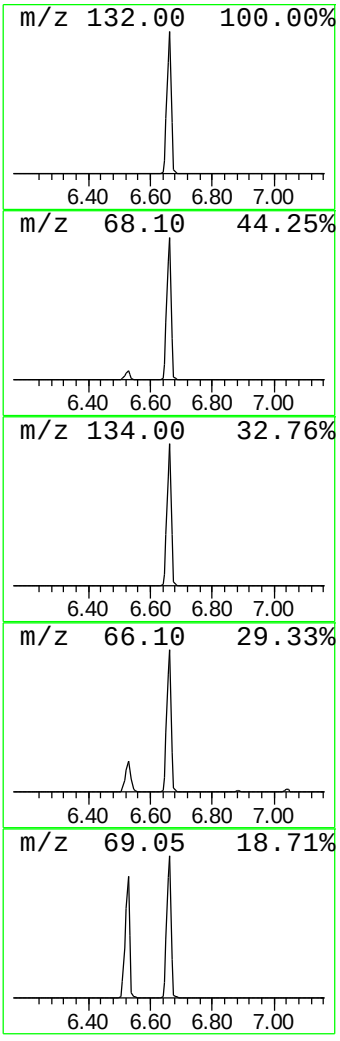
****

Peak Number 4 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	70.67 ng	4167880	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
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





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010919\
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Acq On : 9 Jan 2019 10:45
Operator : JU/SJ
Sample : K1066-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TN-1419

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

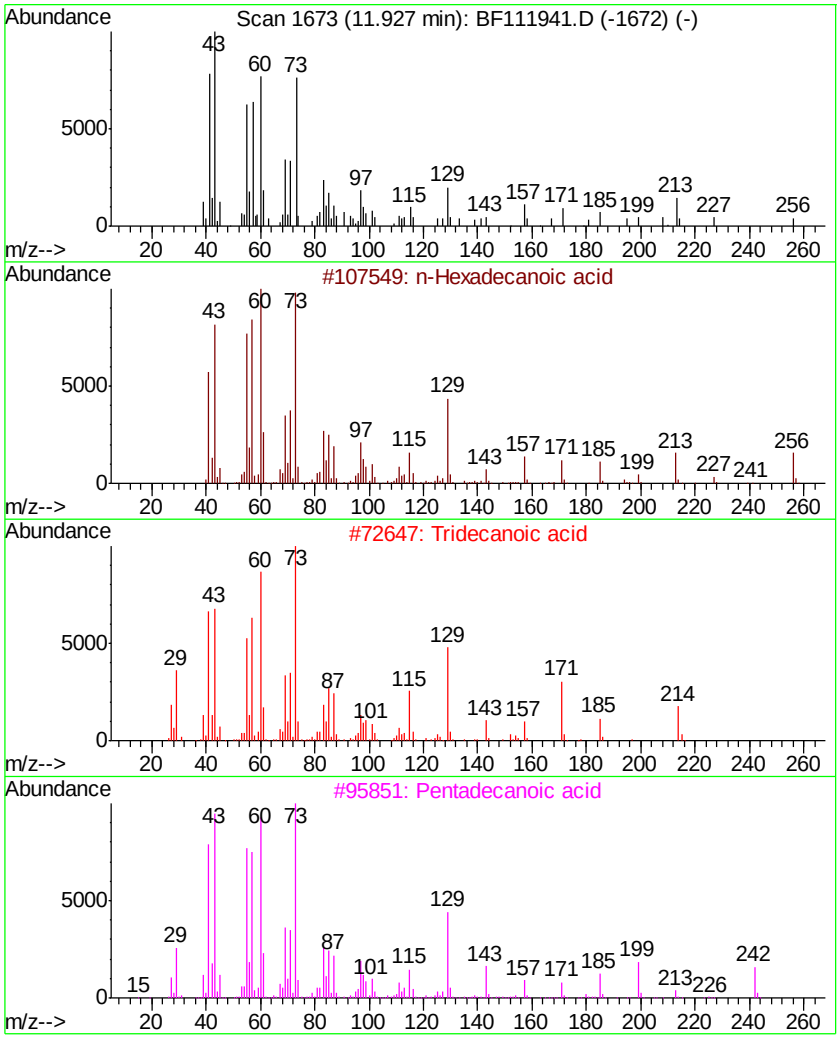
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

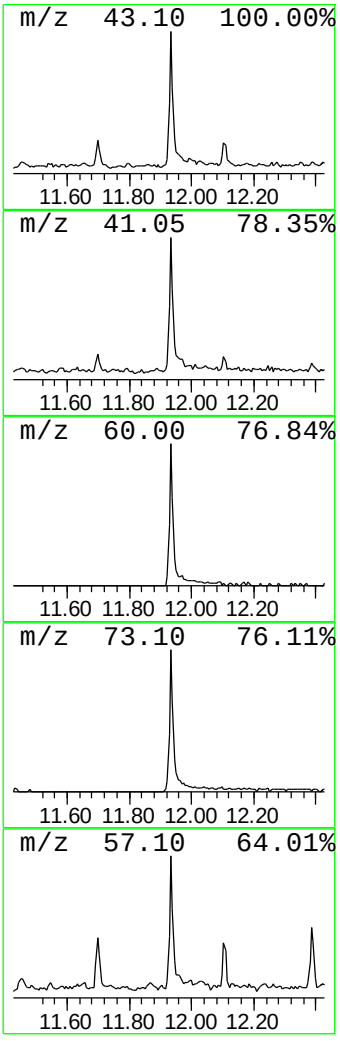
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	2.36 ng	261786	Phenanthrene-d10	11.41

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	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	62
5	Dodecanoic acid	200	C12H24O2	000143-07-7	50





Library Search Compound Report

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Data File : BF111941.D
Acq On : 9 Jan 2019 10:45
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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TN-1419

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

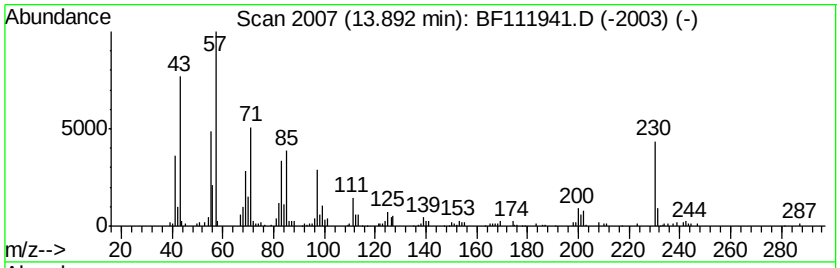
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

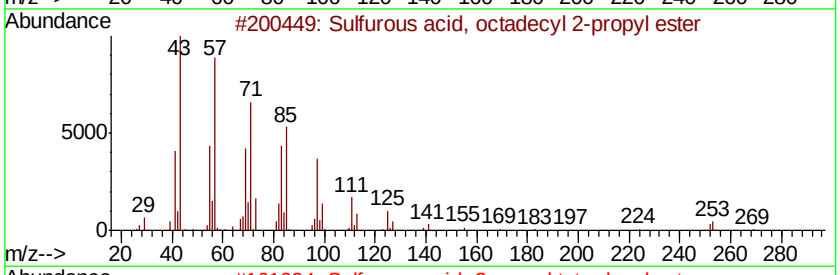
****

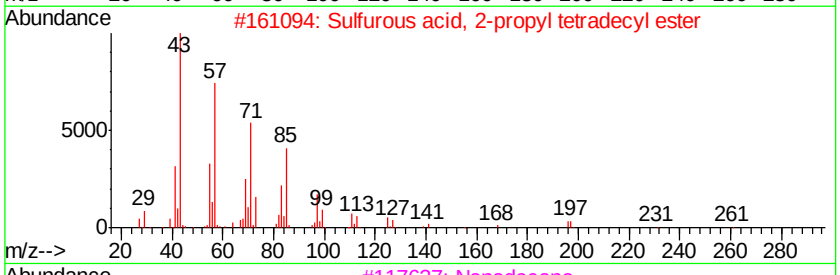
Peak Number 7 Sulfurous acid, octadecyl 2... Concentration Rank 6

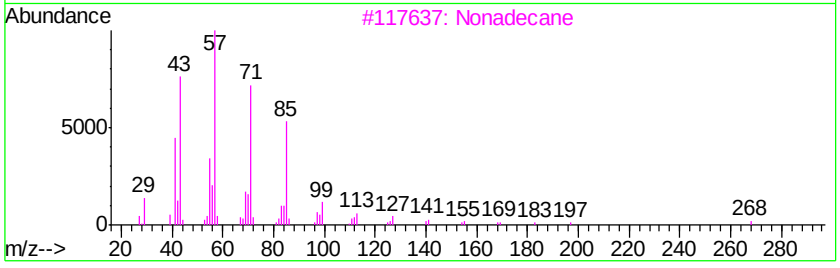
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	2.76 ng	268472	Chrysene-d12	14.05

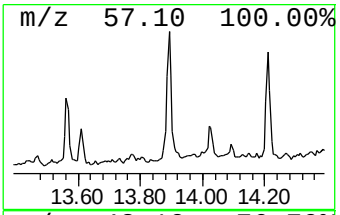
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	70
2	Sulfurous acid, 2-propyl tetrade...	320	C17H36O3S	1000309-12-5	58
3	Nonadecane	268	C19H40	000629-92-5	53
4	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	52
5	Tetradecane	198	C14H30	000629-59-4	49

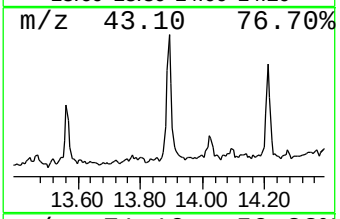


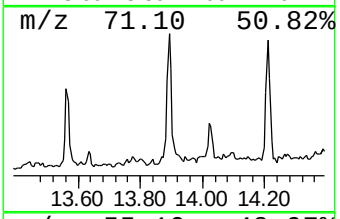


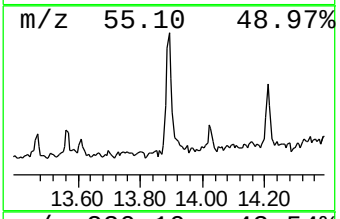


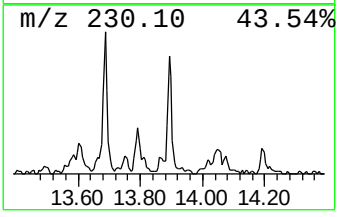












Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010919\
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Sample : K1066-01
Misc :
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Instrument : BNA_F
ClientSampleId : TN-1419

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.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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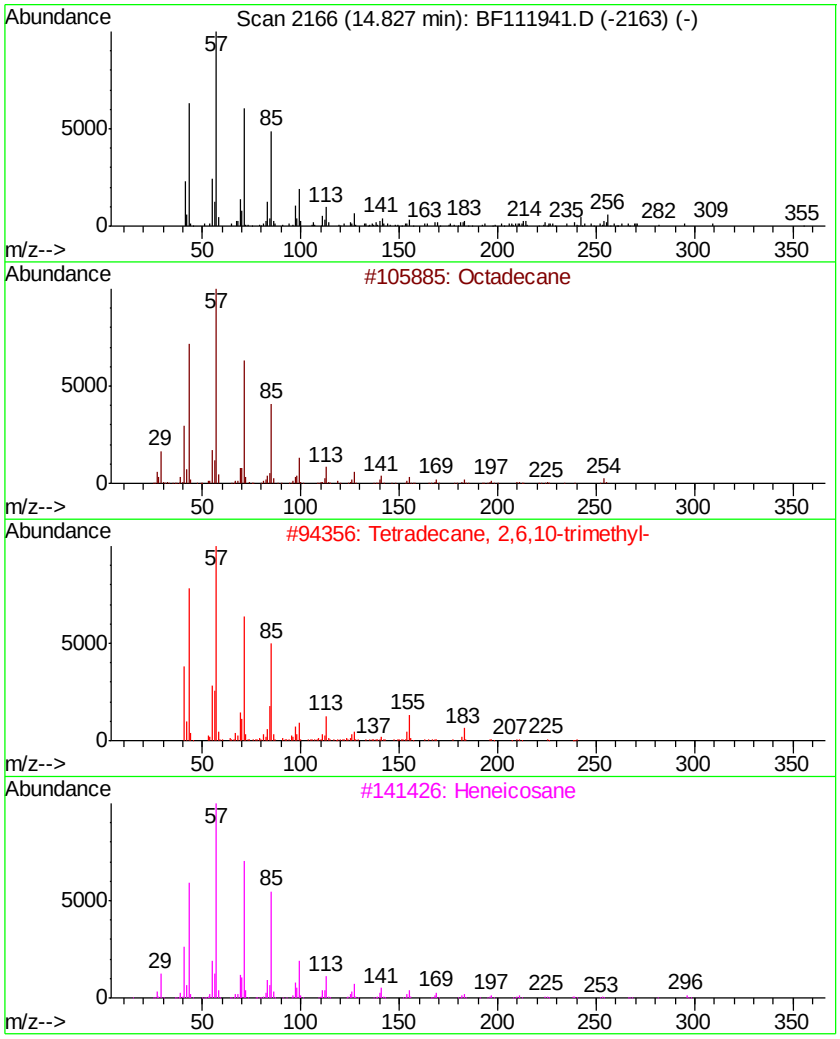
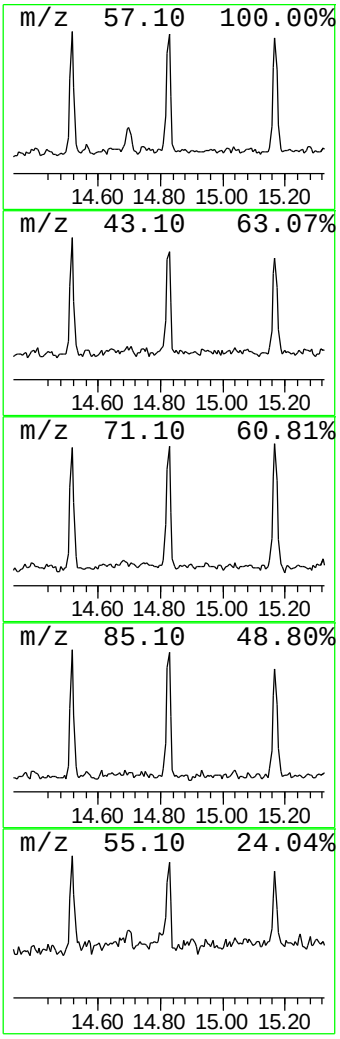
Peak Number 8 Octadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.83	2.32 ng	169448	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	91
2	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	87
3	Heneicosane	296	C21H44	000629-94-7	83
4	Tetracosane	338	C24H50	000646-31-1	80
5	Tetratetracontane	619	C44H90	007098-22-8	76





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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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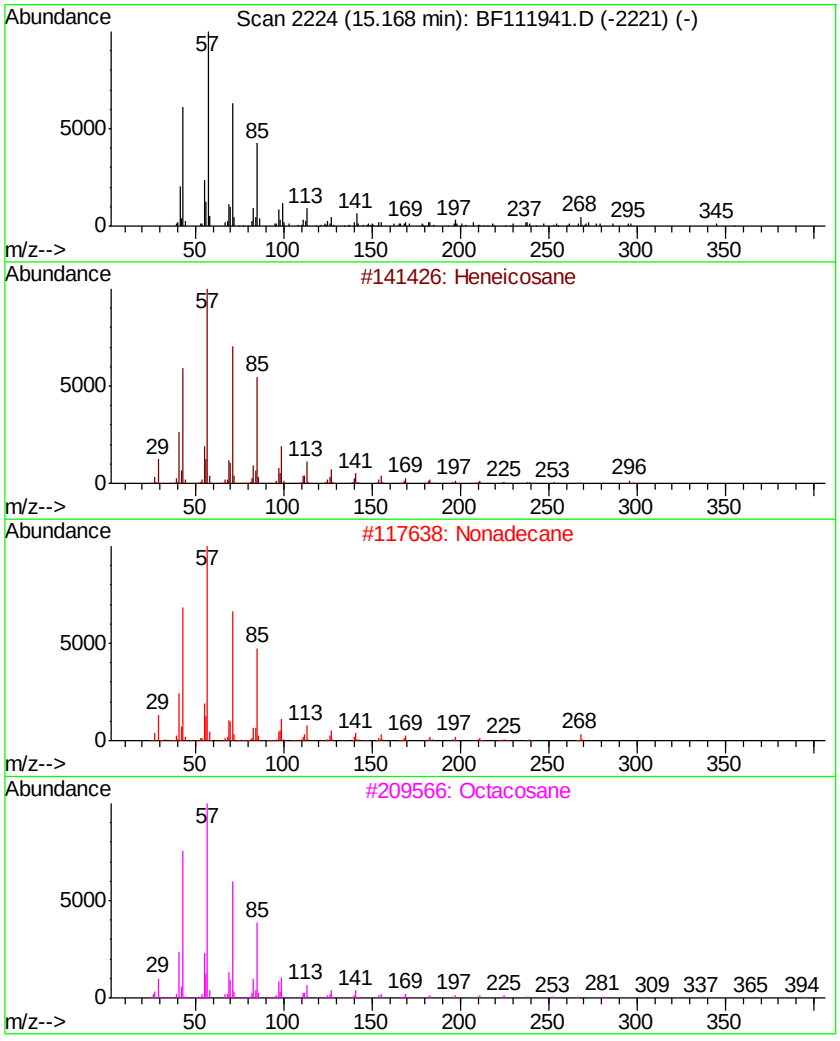
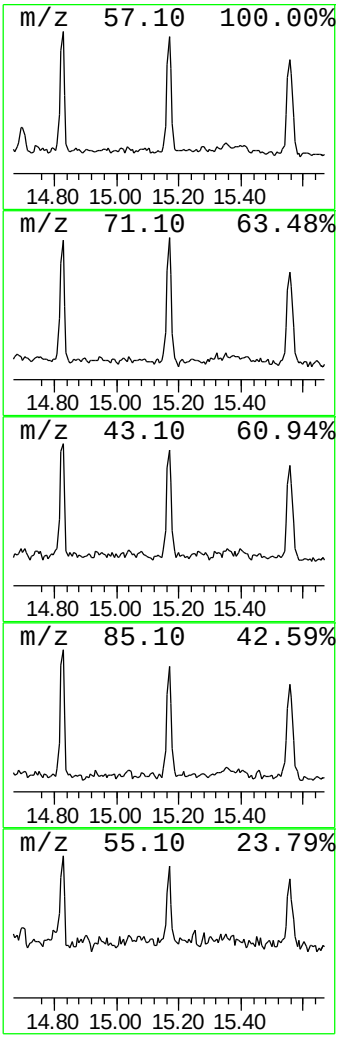
Peak Number 9 Heneicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.17	2.07 ng	151165	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	98
2	Nonadecane	268	C19H40	000629-92-5	93
3	Octacosane	394	C28H58	000630-02-4	87
4	Tetracosane	338	C24H50	000646-31-1	83
5	Heptacosane	380	C27H56	000593-49-7	83





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010919\
Data File : BF111941.D
Acq On : 9 Jan 2019 10:45
Operator : JU/SJ
Sample : K1066-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TN-1419

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.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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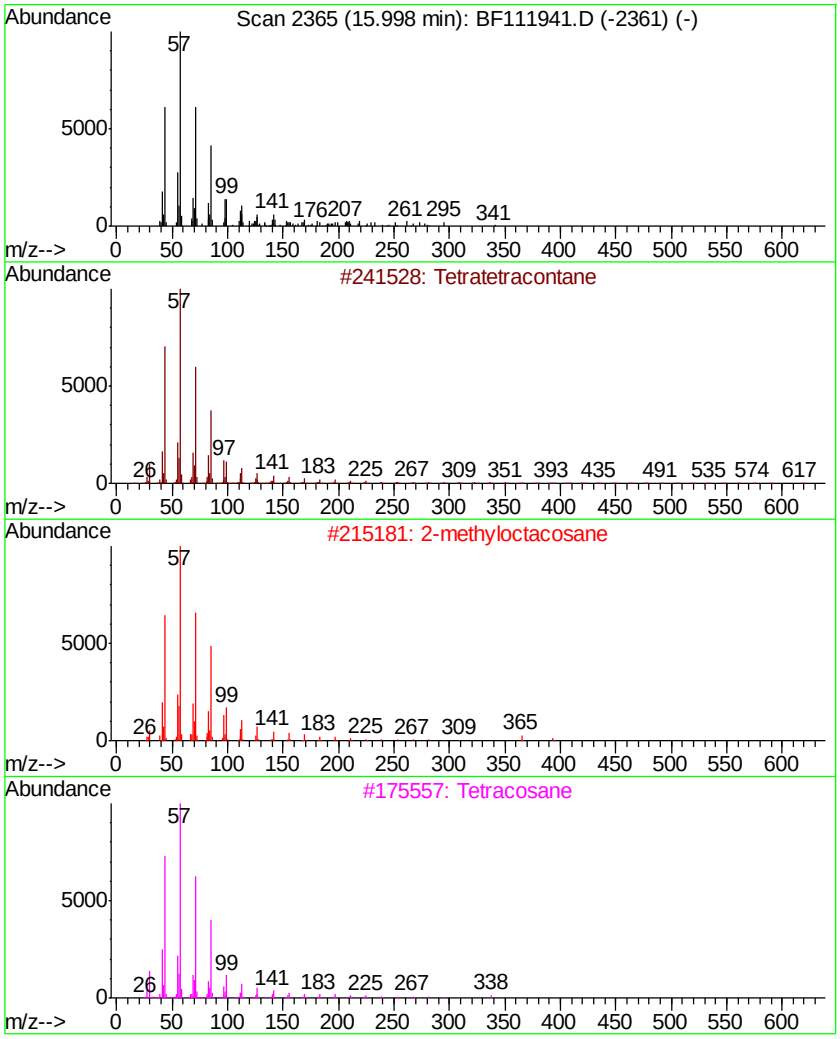
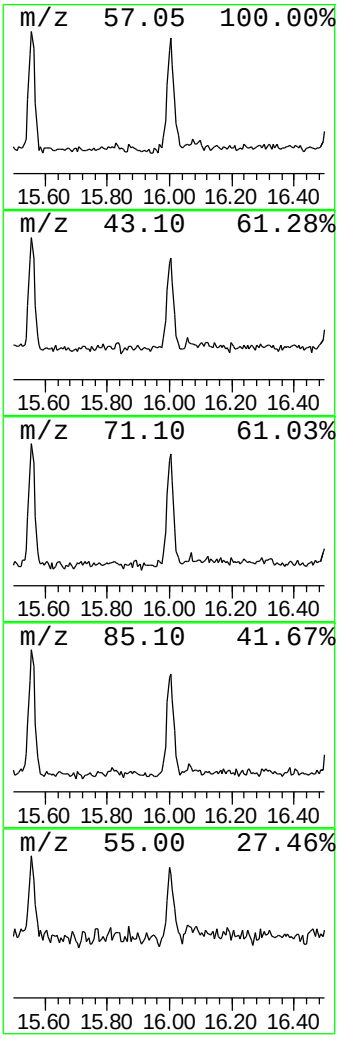
Peak Number 10 Tetratetracontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.00	2.37 ng	173014	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	90
2	2-methyloctacosane	408	C29H60	1000376-72-8	87
3	Tetracosane	338	C24H50	000646-31-1	87
4	Hentriacontane	437	C31H64	000630-04-6	87
5	Hexacosane	366	C26H54	000630-01-3	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF010919\
Data File : BF111941.D
Acq On : 9 Jan 2019 10:45
Operator : JU/SJ
Sample : K1066-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TN-1419

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.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...	2.25	3.7	ng	217415	1	6.89	1179520	20.0
2-Pentanone, 4-hy...	5.12	4.2	ng	249775	1	6.89	1179520	20.0
unknown6.66	6.66	70.7	ng	4167880	1	6.89	1179520	20.0
n-Hexadecanoic acid	11.93	2.4	ng	261786	4	11.41	2214750	20.0
Sulfurous acid, o...	13.89	2.8	ng	268472	5	14.05	1948890	20.0
Octadecane	14.83	2.3	ng	169448	6	15.54	1462760	20.0
Heneicosane	15.17	2.1	ng	151165	6	15.54	1462760	20.0
Tetratetracontane	16.00	2.4	ng	173014	6	15.54	1462760	20.0