LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020719\
Data File : BF112443.D
Acq On : 7 Feb 2019 17:33
Operator : JU/SJ
Sample : K1401-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RT-3451

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-BF012519.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	2.128	3	7	16	rVB	110608	147384	4.60%	0.484%
2	5.057	502	505	513	rBV	103470	143166	4.46%	0.470%
3	5.469	572	575	593	rBV	2886059	2842988	88.65%	9.329%
4	6.416	733	736	743	rVB2	27832	35661	1.11%	0.117%
5	6.487	743	748	761	rBV	2847658	3133877	97.72%	10.283%
6	6.610	765	769	772	rBV	3712837	3206961	100.00%	10.523%
7	6.834	803	807	815	rBV	883524	799912	24.94%	2.625%
8	6.987	829	833	837	rBV	2629913	2399184	74.81%	7.873%
9	7.398	898	903	915	rBV	1985828	1943843	60.61%	6.378%
10	8.116	1021	1025	1036	rBV	1039170	1037561	32.35%	3.405%
11	9.186	1202	1207	1218	rBV	3620347	3172892	98.94%	10.411%
12	9.581	1271	1274	1283	rVB	250856	228708	7.13%	0.750%
13	9.869	1319	1323	1327	rBV	1295277	1123153	35.02%	3.685%
14	9.898	1327	1328	1334	rVB	65803	53811	1.68%	0.177%
15	10.075	1355	1358	1362	rVB	44910	41787	1.30%	0.137%
16	10.416	1413	1416	1422	rVB	71858	68363	2.13%	0.224%
17	10.663	1454	1458	1467	rBV	2232533	2088662	65.13%	6.854%
18	11.357	1572	1576	1578	rBV	1117552	987810	30.80%	3.241%
19	11.380	1578	1580	1586	rVB	301650	261092	8.14%	0.857%
20	11.880	1658	1665	1668	rBV2	201667	263521	8.22%	0.865%
21	11.910	1668	1670	1672	rVB	87057	68091	2.12%	0.223%
22	11.974	1678	1681	1683	rBV	44892	44896	1.40%	0.147%
23	12.574	1779	1783	1788	rBV	237975	227406	7.09%	0.746%
24	12.663	1795	1798	1805	rVB3	35391	40064	1.25%	0.131%
25	12.804	1815	1822	1825	rBV	174125	204907	6.39%	0.672%
26	12.939	1840	1845	1848	rBV	2520409	2350686	73.30%	7.713%
27	13.133	1871	1878	1880	rBV	32022	45641	1.42%	0.150%
28	13.504	1935	1941	1943	rBV4	25234	37638	1.17%	0.124%
29	13.821	1990	1995	2005	rBV4	264317	373750	11.65%	1.226%
30	13.963	2016	2019	2021	rBV	68813	58639	1.83%	0.192%
31	13.998	2021	2025	2028	rVV	887423	931685	29.05%	3.057%
32	14.027	2028	2030	2033	rVB	99187	83918	2.62%	0.275%
33	14.145	2047	2050	2057	rBV2	63757	80293	2.50%	0.263%
34	14.392	2088	2092	2094	rBV	35290	38429	1.20%	0.126%

LSC Area Percent Report

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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RT-3451

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-BF012519.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.451	2095	2102	2110	rVV5	104765	181192	5.65%	0.595%
36	14.751	2150	2153	2156	rVB	99507	92926	2.90%	0.305%
37	14.827	2162	2166	2173	rVB	276722	283444	8.84%	0.930%
38	15.045	2199	2203	2206	rBV	77265	113078	3.53%	0.371%
39	15.080	2206	2209	2213	rVB2	99566	132061	4.12%	0.433%
40	15.345	2251	2254	2258	rVB	50515	65641	2.05%	0.215%
41	15.410	2262	2265	2269	rVV	54495	63432	1.98%	0.208%
42	15.468	2269	2275	2288	rVB2	593166	871338	27.17%	2.859%
43	15.886	2342	2346	2351	rBV2	80053	105959	3.30%	0.348%

Sum of corrected areas: 30475450

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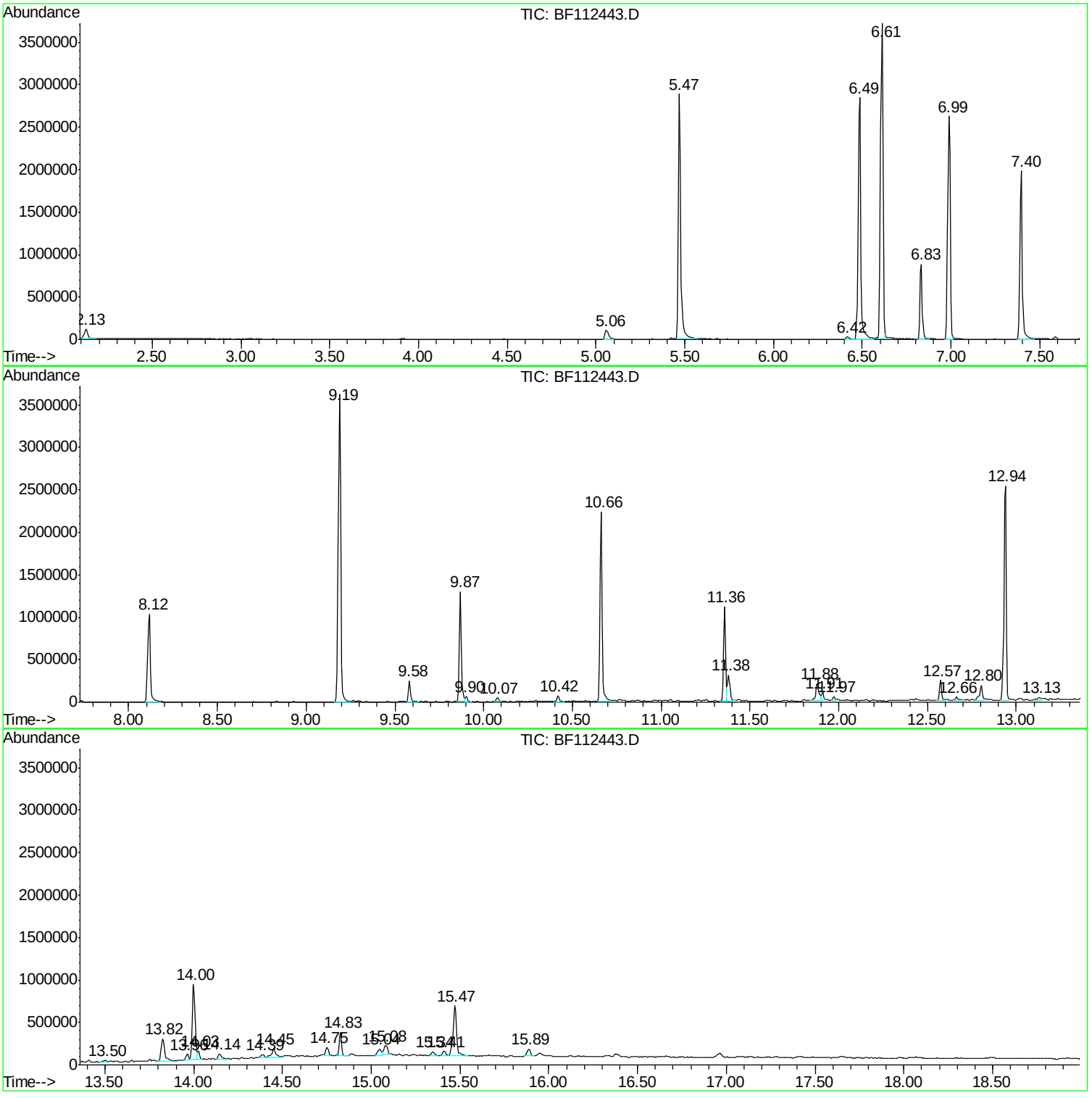
Instrument :
BNA_F
ClientSampleId :
RT-3451

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.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 : BF112443.D
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ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.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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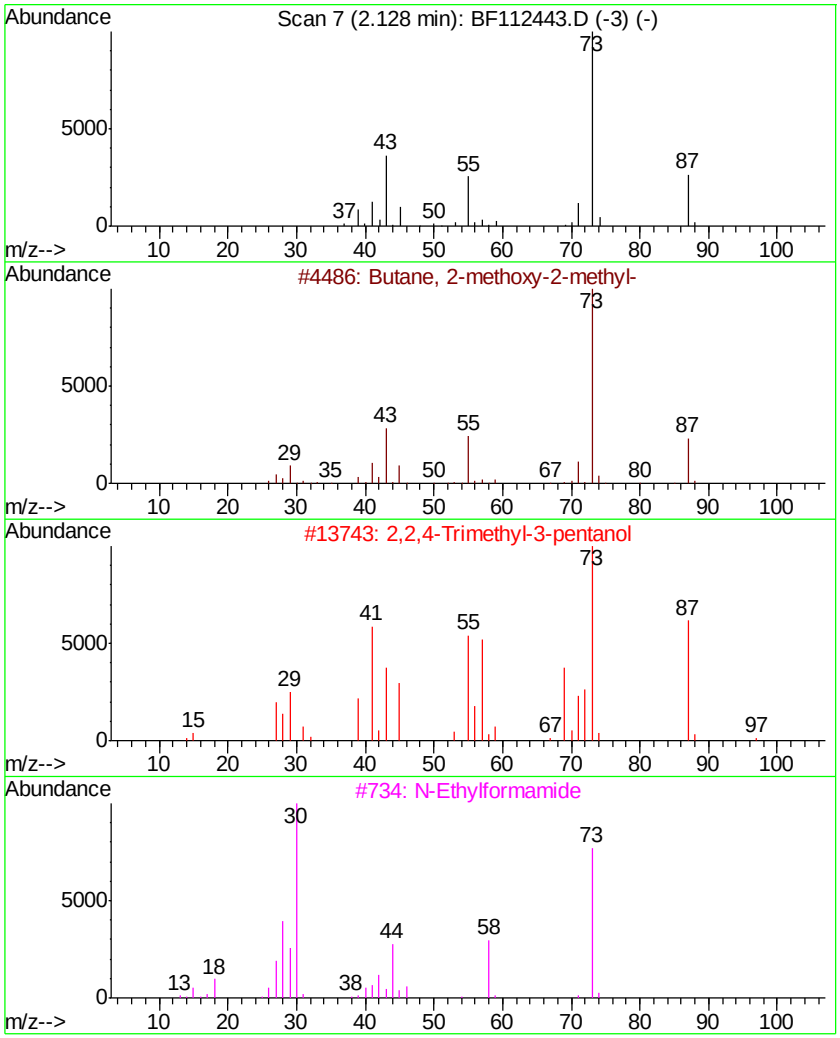
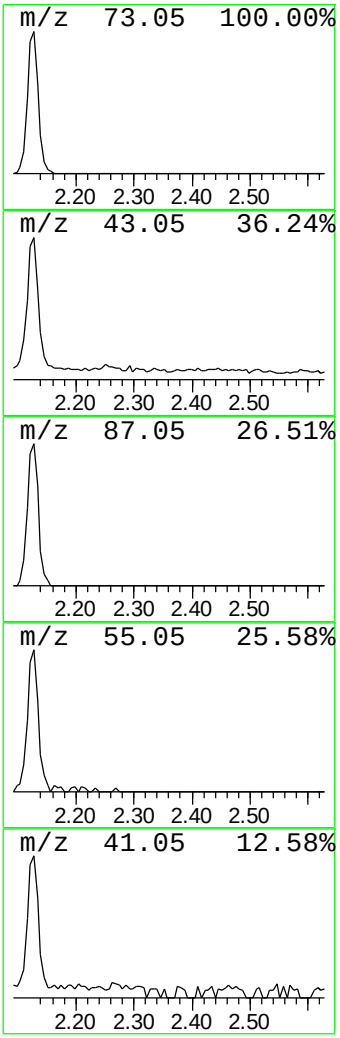
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.13	3.69 ng	147384	1,4-Dichlorobenzene-d4	6.83

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	N-Ethylformamide	73	C3H7NO	000627-45-2	9
4	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	9
5	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	9





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Instrument : BNA_F
ClientSampleId : RT-3451

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.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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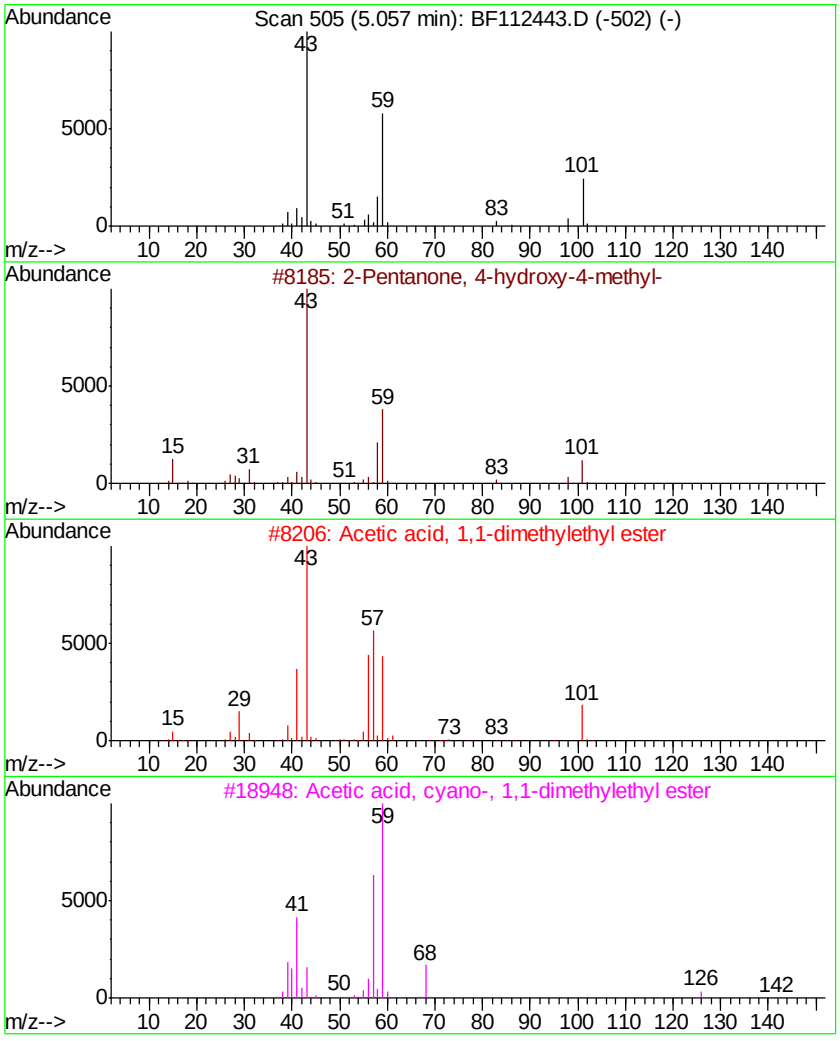
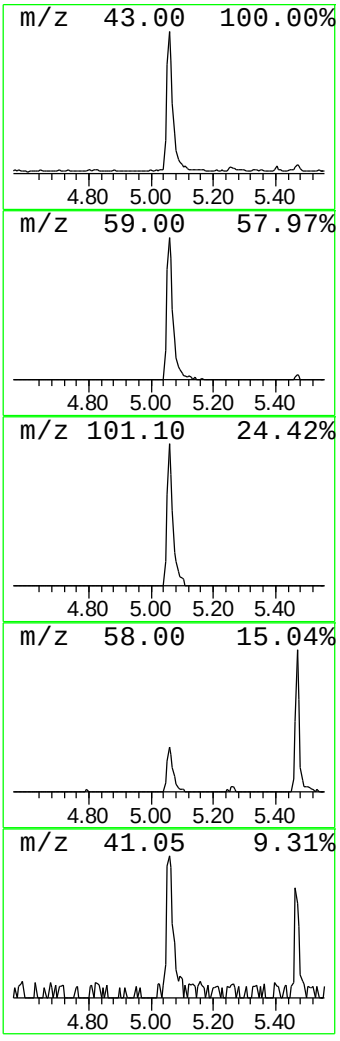
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	3.58 ng	143166	1,4-Dichlorobenzene-d4	6.83

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	17
5	Guanidine	59	CH5N3	000113-00-8	9





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Sample : K1401-07
Misc :
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Instrument : BNA_F
ClientSampleId : RT-3451

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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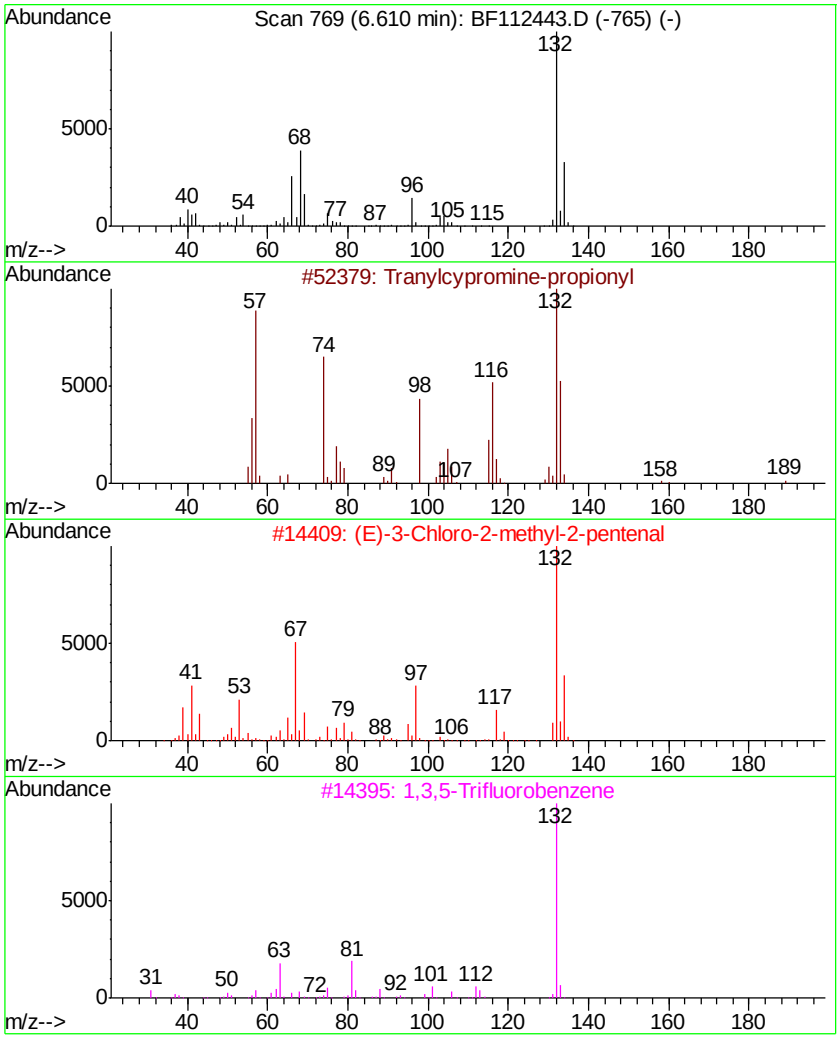
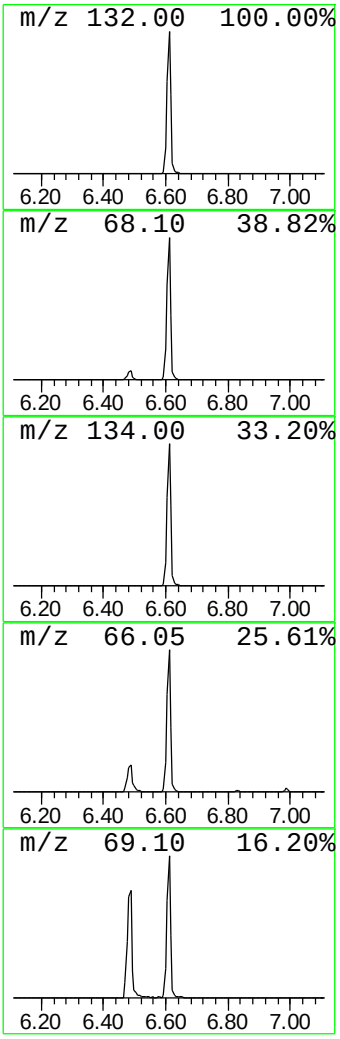
Peak Number 3 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	80.18 ng	3206960	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4	Xenon	132	Xe	007440-63-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Library Search Compound Report

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Instrument : BNA_F
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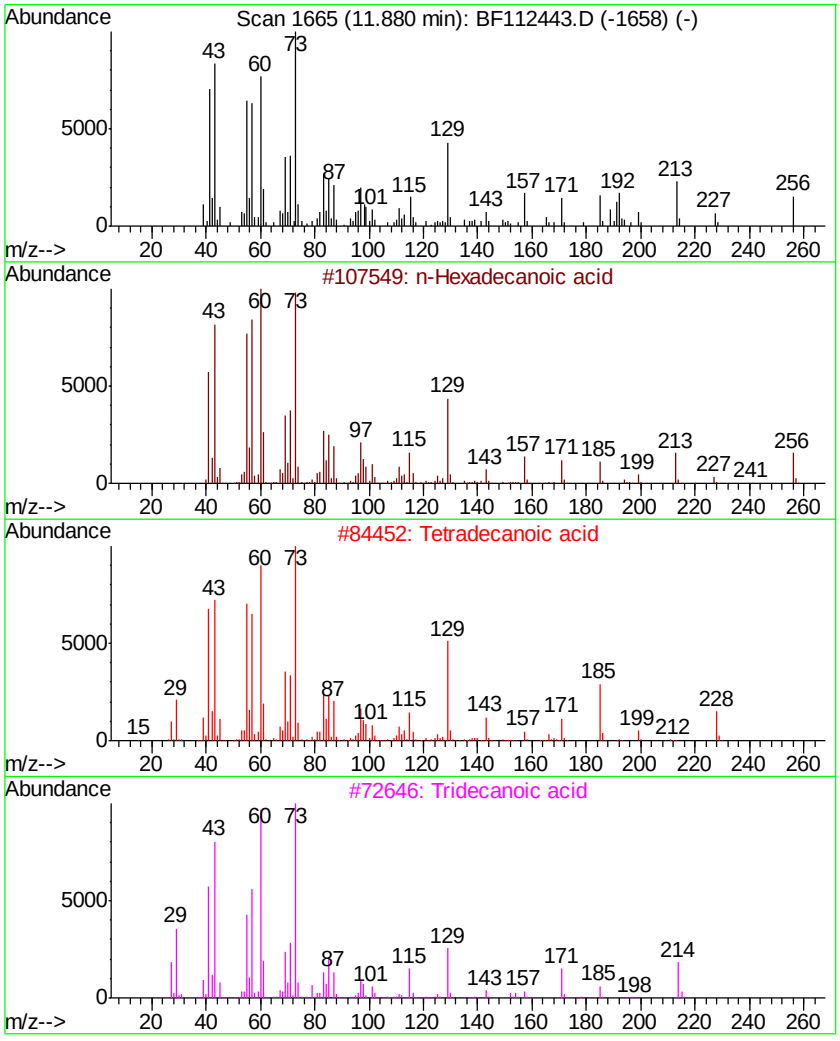
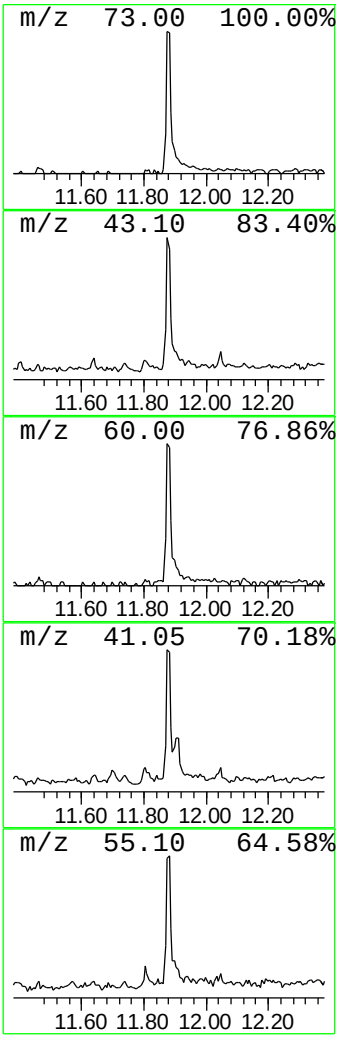
Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.88	5.34 ng	263521	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	89
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70





Library Search Compound Report

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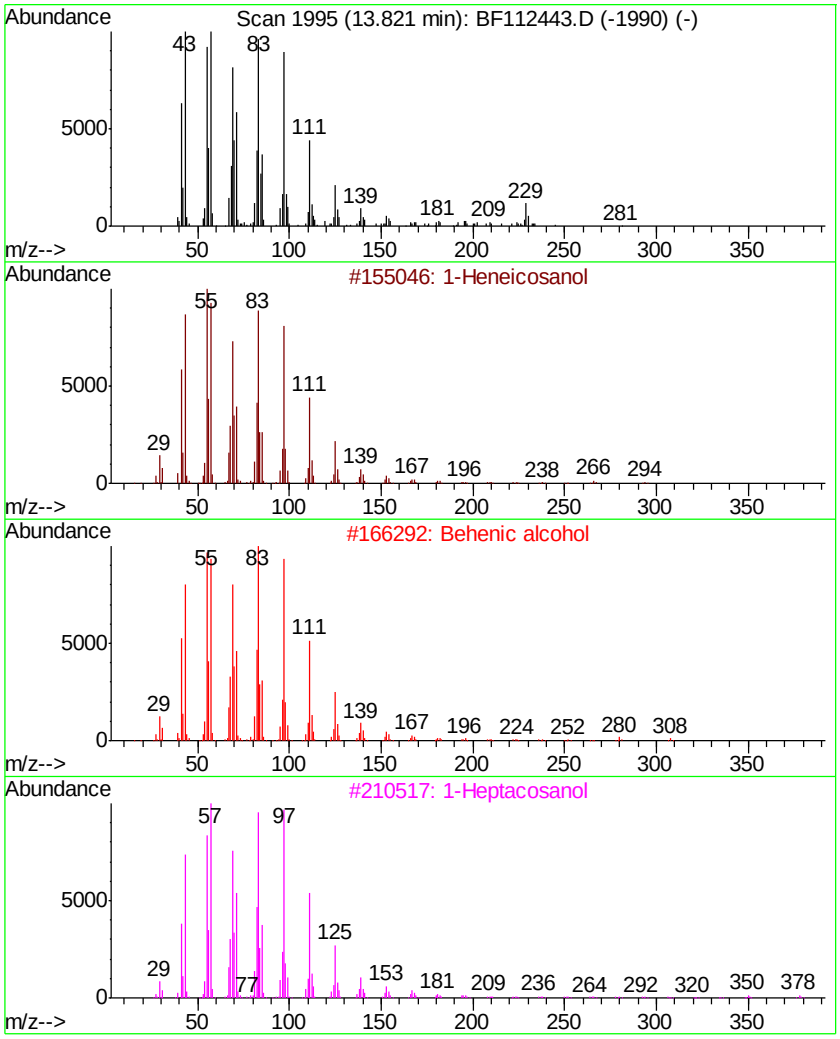
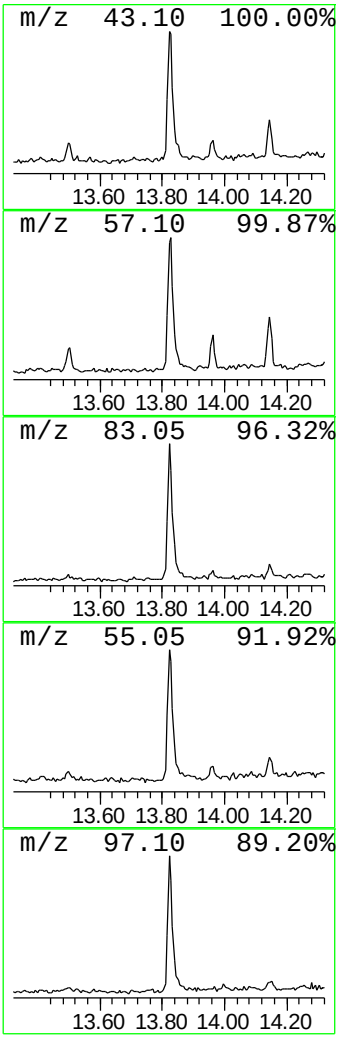
Peak Number 6 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	8.02 ng	373750	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Behenic alcohol	326	C22H46O	000661-19-8	95
3	1-Heptacosanol	396	C27H56O	002004-39-9	94
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	91





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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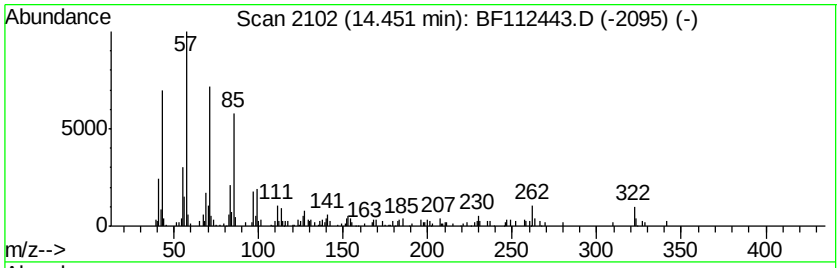
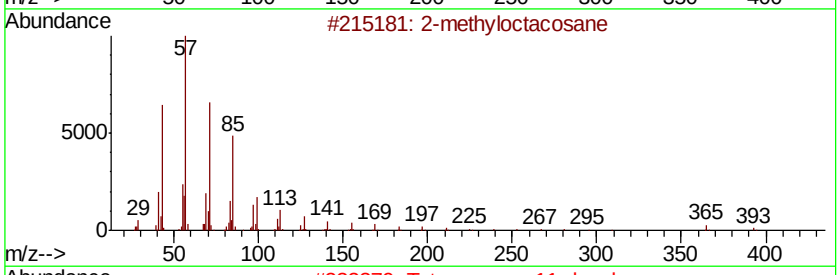
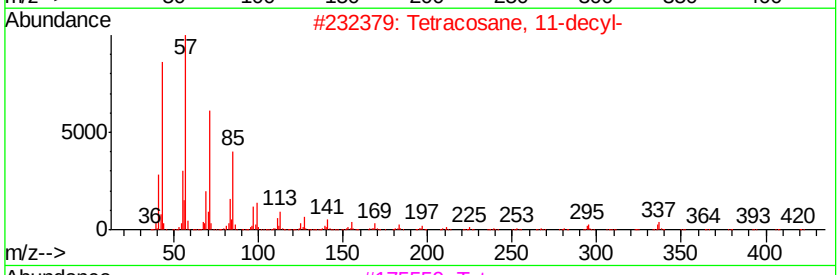
Peak Number 7 2-methyloctacosane Concentration Rank 6

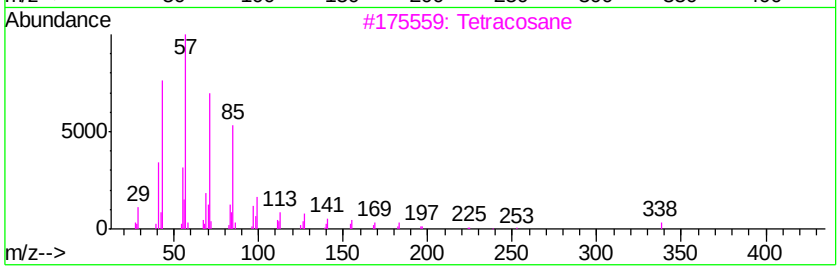
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.45	3.89 ng	181192	Chrysene-d12	14.00

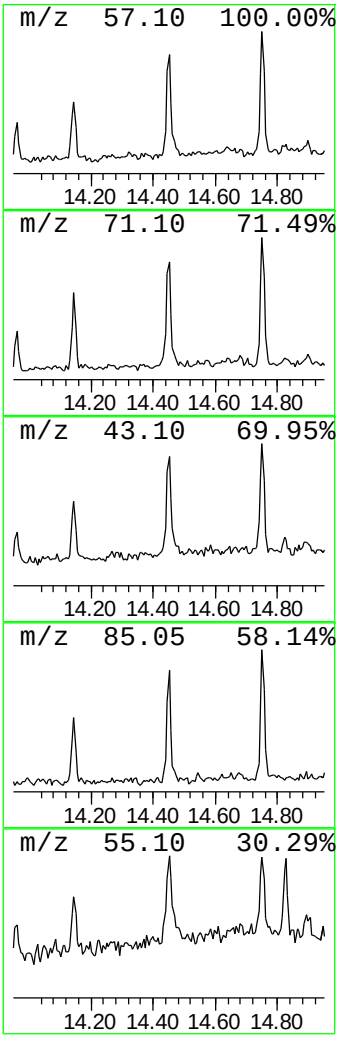
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	62
2	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	62
3	Tetracosane	338	C24H50	000646-31-1	62
4	Hexacosane	366	C26H54	000630-01-3	62
5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	58











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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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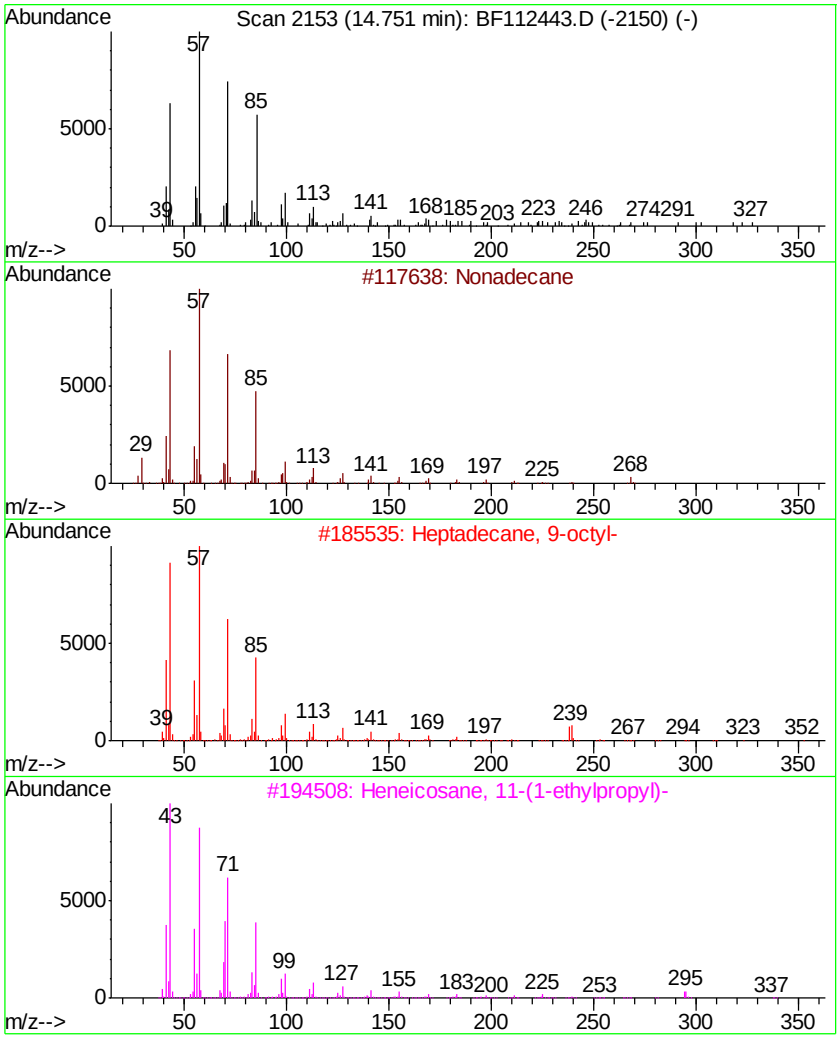
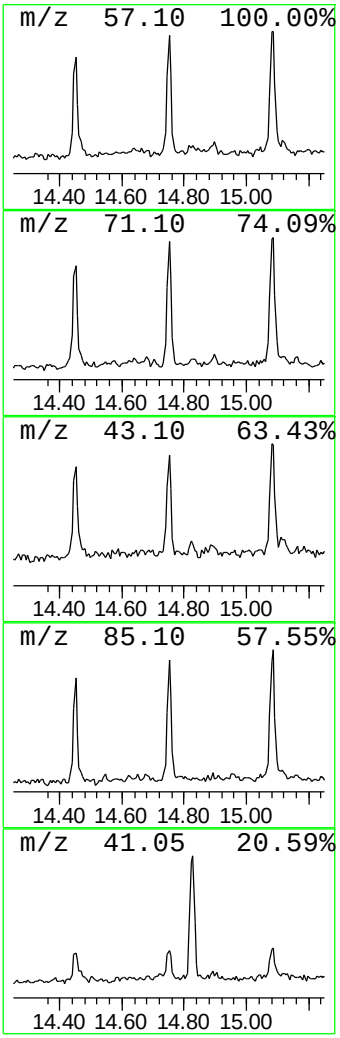
Peak Number 8 Nonadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.75	2.13 ng	92926	Perylene-d12	15.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	93
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	2-methyloctacosane	408	C29H60	1000376-72-8	91





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TIC Library : C:\DATABASE\NIST11.L
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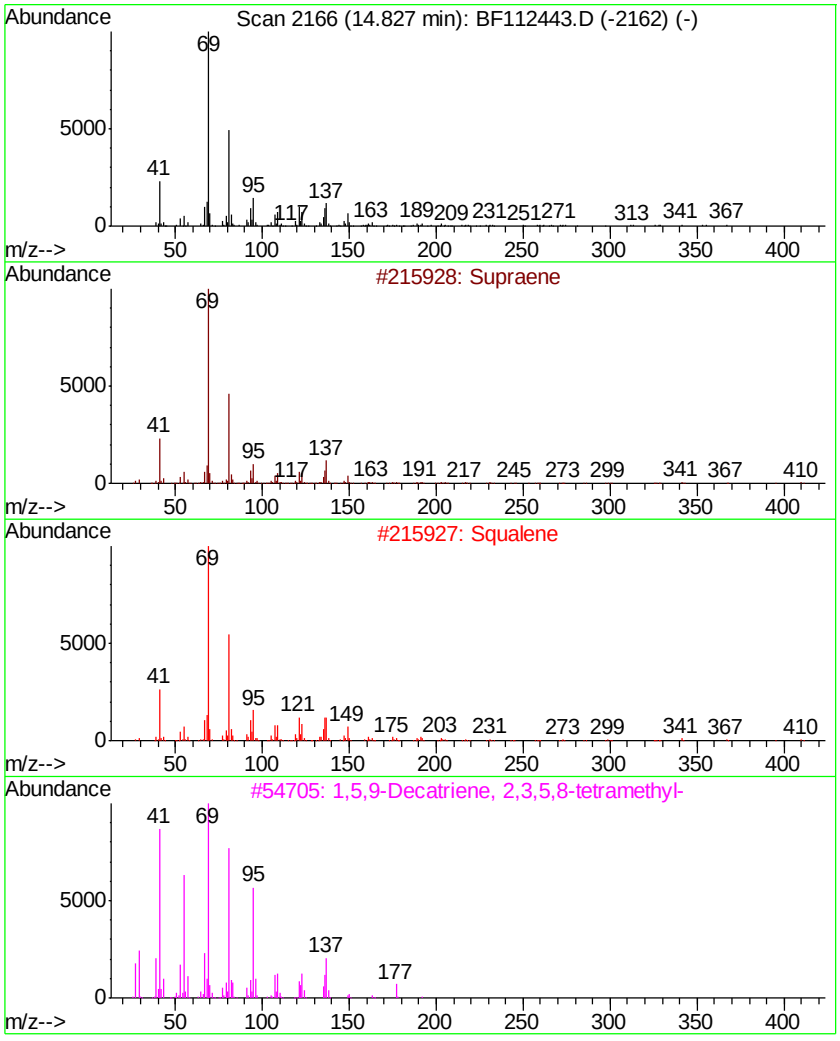
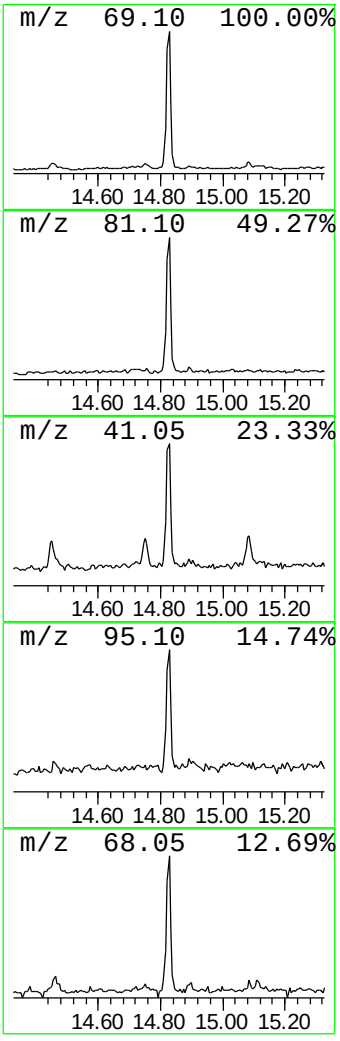
Peak Number 9 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.83	6.51 ng	283444	Perylene-d12	15.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	Squalene	410	C30H50	000111-02-4	91
3	1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	80
4	trans-Farnesol	222	C15H26O	000106-28-5	78
5	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	78





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020719\
Data File : BF112443.D
Acq On : 7 Feb 2019 17:33
Operator : JU/SJ
Sample : K1401-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RT-3451

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

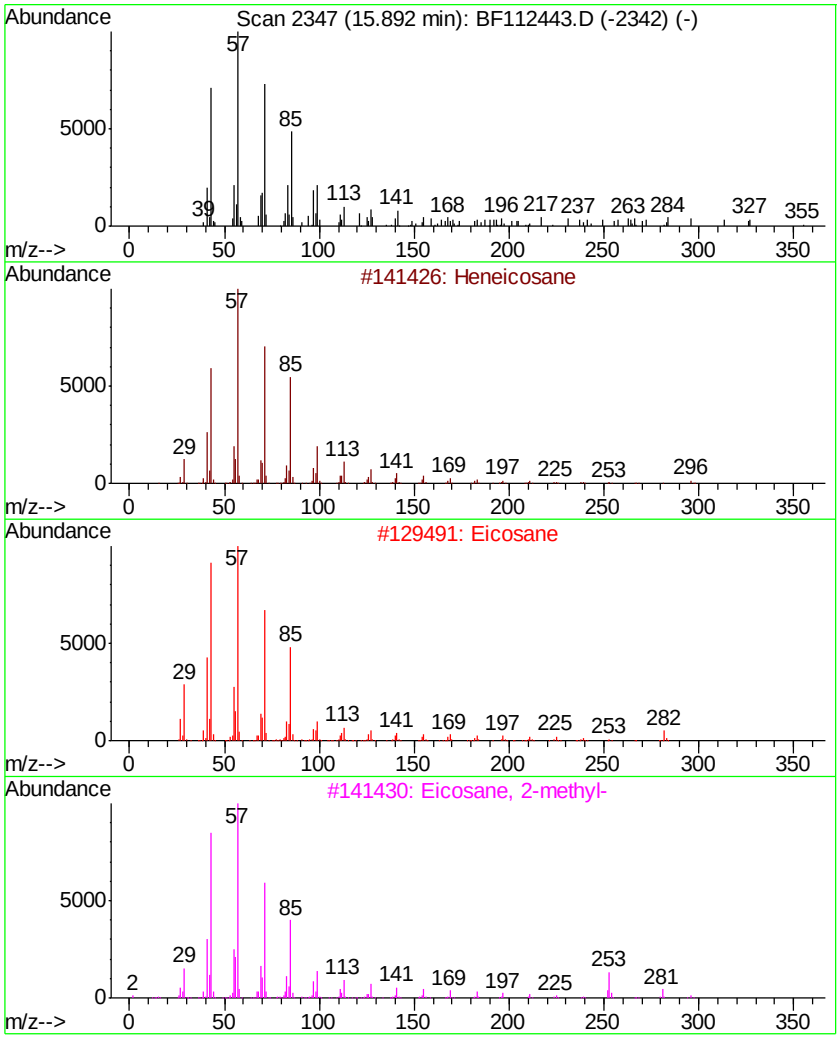
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

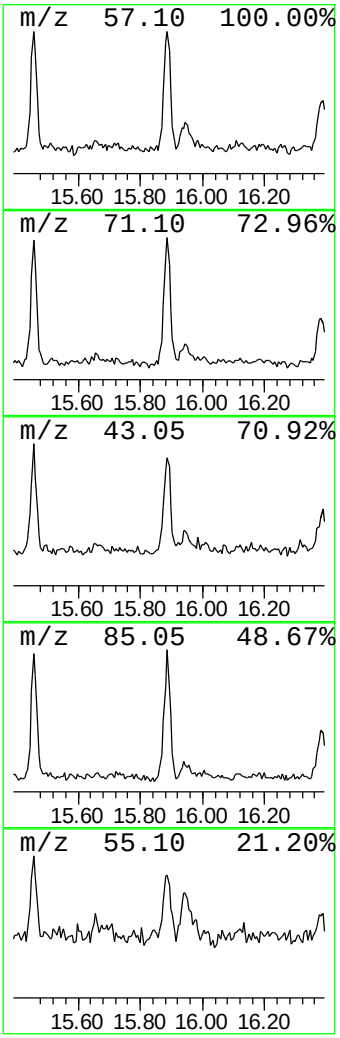
****

Peak Number 10 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.89	2.43 ng	105959	Perylene-d12	15.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	99
2	Eicosane	282	C20H42	000112-95-8	94
3	Eicosane, 2-methyl-	296	C21H44	001560-84-5	93
4	2-methyloctacosane	408	C29H60	1000376-72-8	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF020719\
Data File : BF112443.D
Acq On : 7 Feb 2019 17:33
Operator : JU/SJ
Sample : K1401-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RT-3451

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.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...	2.13	3.7	ng	147384	1	6.83	799912	20.0
2-Pentanone, 4-hy...	5.06	3.6	ng	143166	1	6.83	799912	20.0
unknown6.61	6.61	80.2	ng	3206960	1	6.83	799912	20.0
n-Hexadecanoic acid	11.88	5.3	ng	263521	4	11.36	987810	20.0
1-Heneicosanol	13.82	8.0	ng	373750	5	14.00	931685	20.0
2-methyloctacosane	14.45	3.9	ng	181192	5	14.00	931685	20.0
Nonadecane	14.75	2.1	ng	92926	6	15.47	871338	20.0
Supraene	14.83	6.5	ng	283444	6	15.47	871338	20.0
Heneicosane	15.89	2.4	ng	105959	6	15.47	871338	20.0