LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110218\
Data File : BF110434.D
Acq On : 3 Nov 2018 1:32
Operator : JU/SJ
Sample : J5769-17
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GOFFLE-RD-2

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-BF102318.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	2.287	29	34	51	rVB	311519	451588	23.57%	2.567%
2	5.198	525	529	538	rBV	56822	73187	3.82%	0.416%
3	5.581	590	594	613	rBV	1832494	1764664	92.11%	10.031%
4	6.581	759	764	784	rVB	1716684	1915781	100.00%	10.890%
5	6.728	784	789	792	rBV	2067128	1844336	96.27%	10.483%
6	6.957	824	828	834	rBV	556523	487617	25.45%	2.772%
7	7.110	850	854	858	rBV	1580406	1426259	74.45%	8.107%
8	7.516	919	923	934	rBV	1073839	1081295	56.44%	6.146%
9	8.239	1042	1046	1060	rBV	561313	576956	30.12%	3.279%
10	9.310	1224	1228	1238	rBV	2240420	1845434	96.33%	10.490%
11	9.704	1291	1295	1301	rBV	189907	183577	9.58%	1.043%
12	9.998	1341	1345	1357	rVB	621255	564073	29.44%	3.206%
13	10.786	1475	1479	1489	rBV	953245	920425	48.04%	5.232%
14	11.486	1595	1598	1601	rBV	519854	506067	26.42%	2.877%
15	11.510	1601	1602	1607	rVB	102295	84878	4.43%	0.482%
16	11.992	1680	1684	1687	rBV	76845	72360	3.78%	0.411%
17	12.022	1687	1689	1693	rVB2	25147	25421	1.33%	0.144%
18	12.104	1700	1703	1706	rBV2	30330	40274	2.10%	0.229%
19	12.545	1774	1778	1780	rBV2	19131	28836	1.51%	0.164%
20	12.704	1802	1805	1809	rBV	316190	293898	15.34%	1.671%
21	12.939	1838	1845	1850	rVB	209787	266722	13.92%	1.516%
22	12.998	1850	1855	1860	rBV5	25555	37183	1.94%	0.211%
23	13.069	1863	1867	1870	rBV	1653550	1407170	73.45%	7.999%
24	13.157	1877	1882	1885	rBV3	16200	26179	1.37%	0.149%
25	13.239	1892	1896	1897	rBV4	20213	21456	1.12%	0.122%
26	13.263	1897	1900	1901	rVV	31230	25286	1.32%	0.144%
27	13.498	1937	1940	1942	rBV2	29194	28426	1.48%	0.162%
28	13.616	1958	1960	1963	rBV3	28661	27942	1.46%	0.159%
29	13.951	2013	2017	2020	rBV2	134231	154528	8.07%	0.878%
30	13.986	2020	2023	2026	rVB	29777	32838	1.71%	0.187%
31	14.133	2043	2048	2051	rBV2	444210	511190	26.68%	2.906%
32	14.163	2051	2053	2057	rVB	89357	84092	4.39%	0.478%
33	14.263	2068	2070	2072	rVB	34691	27909	1.46%	0.159%
34	14.568	2120	2122	2128	rVB	50549	56815	2.97%	0.323%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110218\
Data File : BF110434.D
Acq On : 3 Nov 2018 1:32
Operator : JU/SJ
Sample : J5769-17
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GOFFLE-RD-2

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-BF102318.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.886	2173	2176	2179	rVB	58983	58088	3.03%	0.330%
36	14.968	2187	2190	2195	rVB	73539	80209	4.19%	0.456%
37	15.210	2228	2231	2233	rBV	44662	62472	3.26%	0.355%
38	15.239	2233	2236	2241	rVB2	76020	89732	4.68%	0.510%
39	15.598	2293	2297	2300	rBV	58908	85790	4.48%	0.488%
40	15.663	2301	2308	2312	rVB	187126	321941	16.80%	1.830%

Sum of corrected areas: 17592894

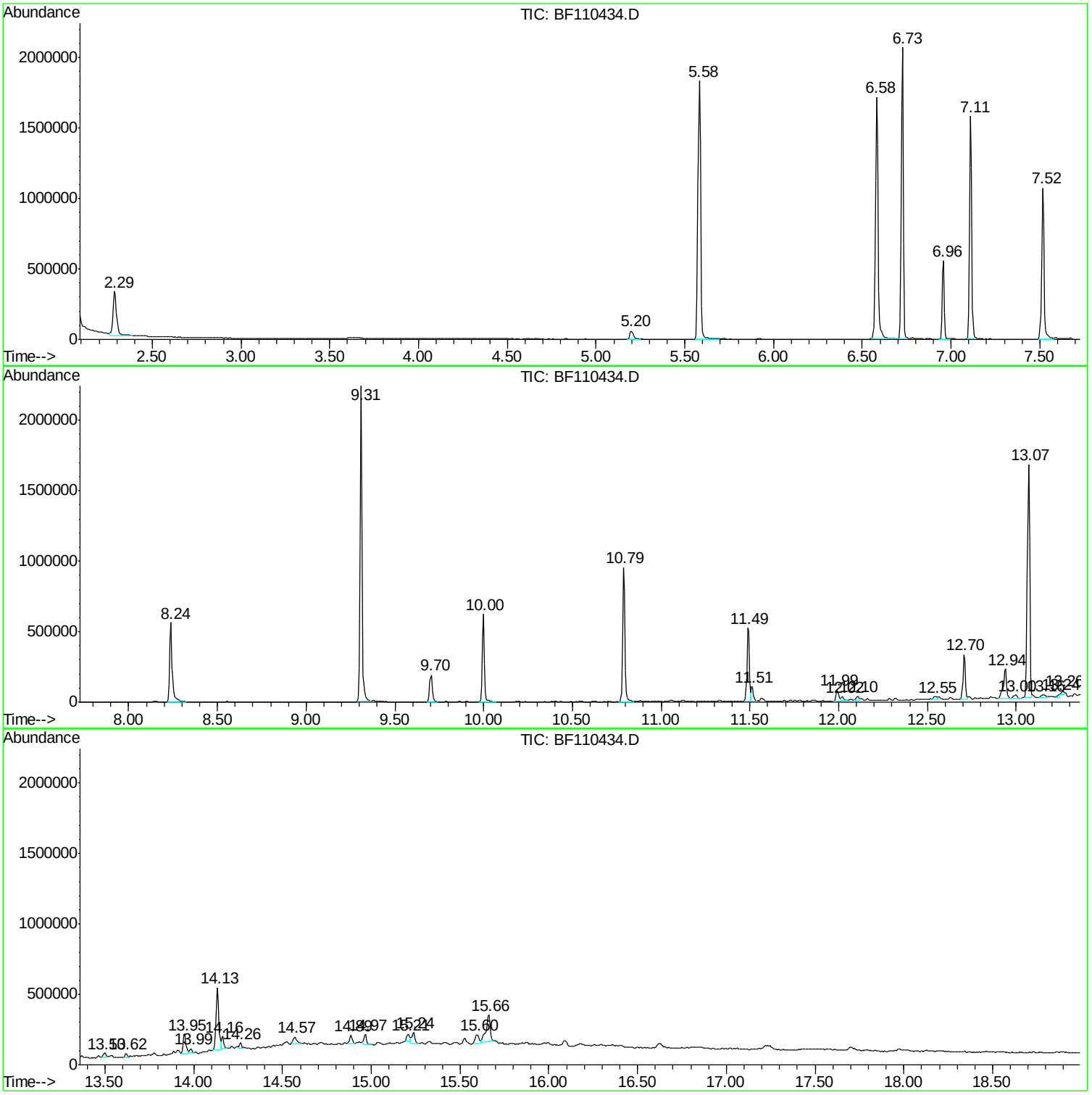
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110218\
Data File : BF110434.D
Acq On : 3 Nov 2018 1:32
Operator : JU/SJ
Sample : J5769-17
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GOFFLE-RD-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.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\BF110218\
Data File : BF110434.D
Acq On : 3 Nov 2018 1:32
Operator : JU/SJ
Sample : J5769-17
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GOFFLE-RD-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

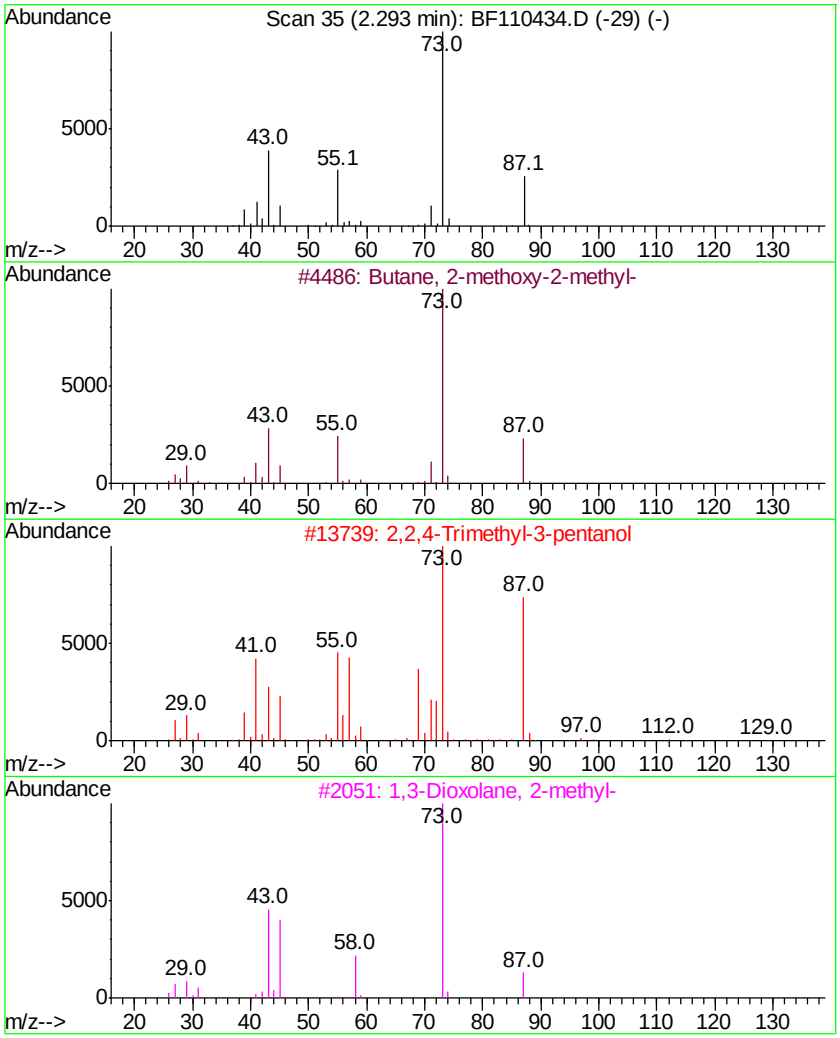
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

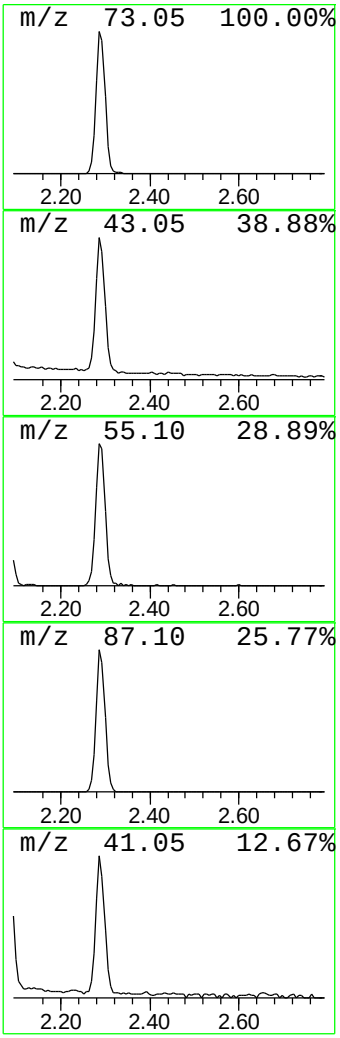
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.29	18.52 ng	451588	1,4-Dichlorobenzene-d4	6.96

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	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	12
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110218\
Data File : BF110434.D
Acq On : 3 Nov 2018 1:32
Operator : JU/SJ
Sample : J5769-17
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GOFFLE-RD-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

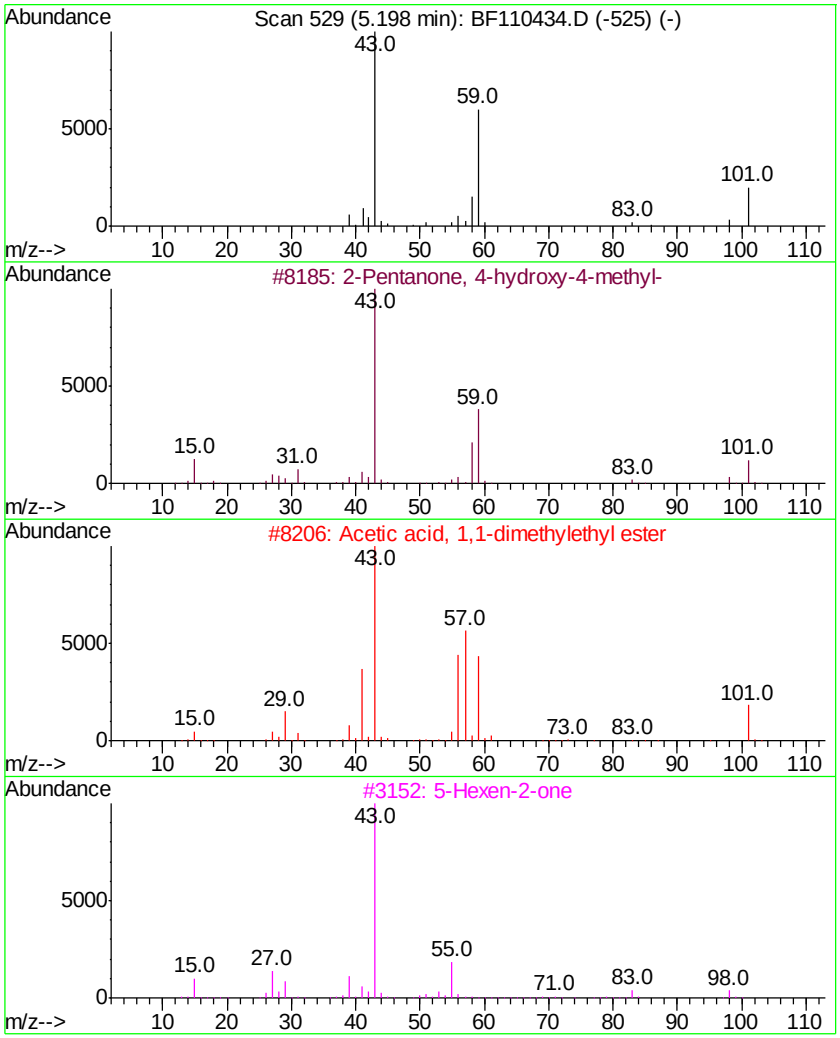
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

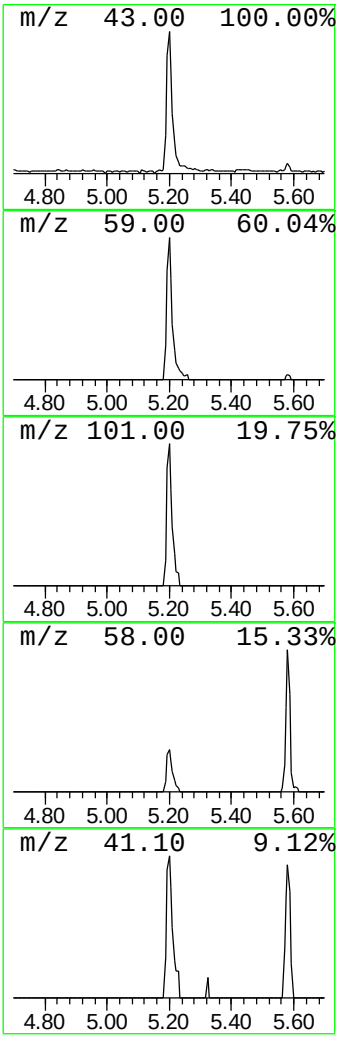
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	3.00 ng	73187	1,4-Dichlorobenzene-d4	6.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110218\
Data File : BF110434.D
Acq On : 3 Nov 2018 1:32
Operator : JU/SJ
Sample : J5769-17
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GOFFLE-RD-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

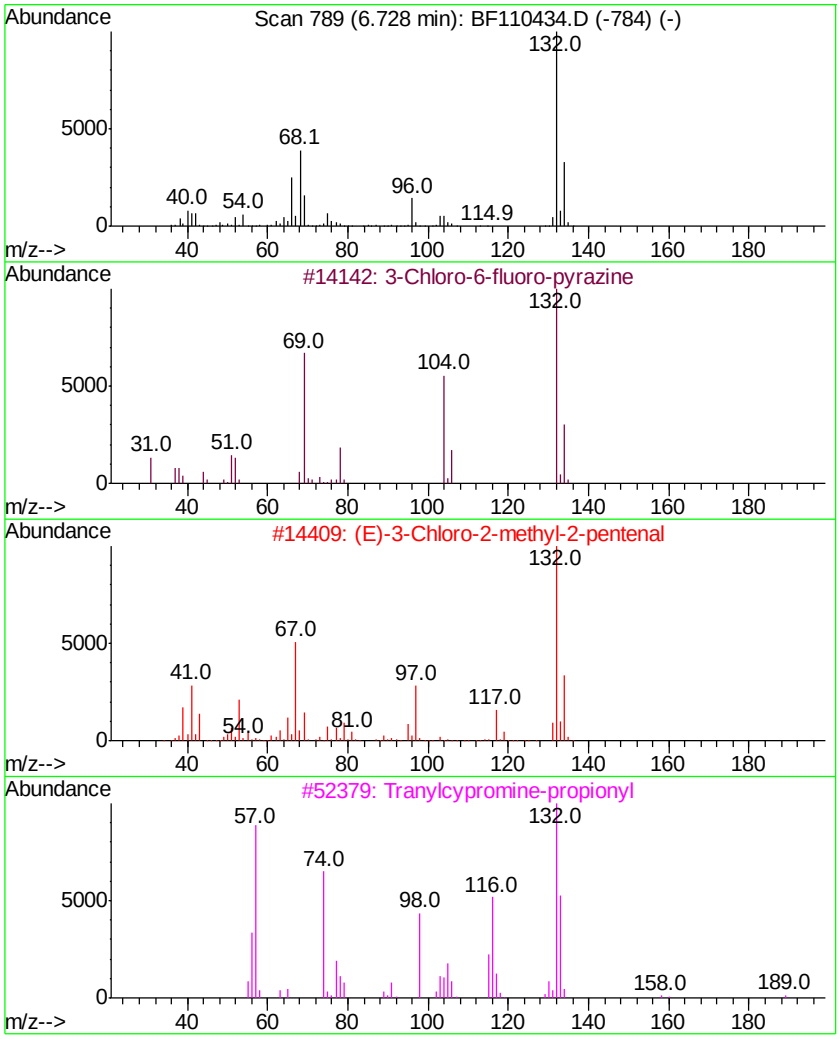
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

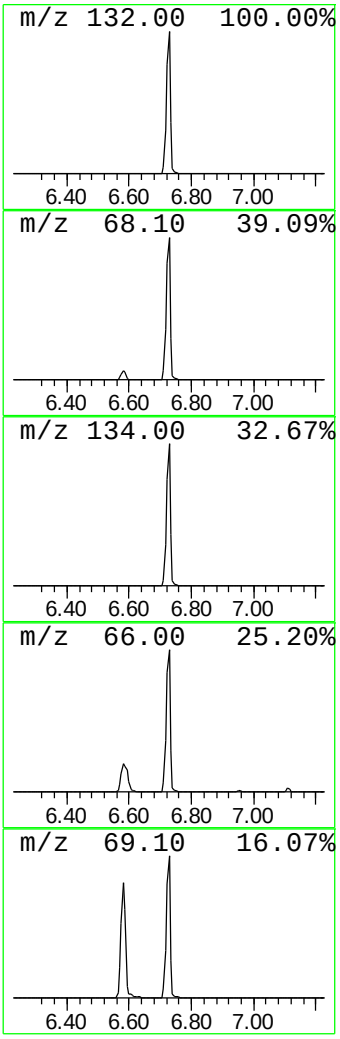
****

Peak Number 3 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	75.65 ng	1844340	1,4-Dichlorobenzene-d4	6.96

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	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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Sample : J5769-17
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GOFFLE-RD-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
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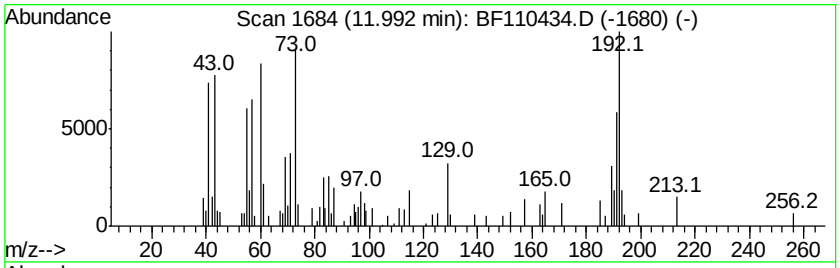
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

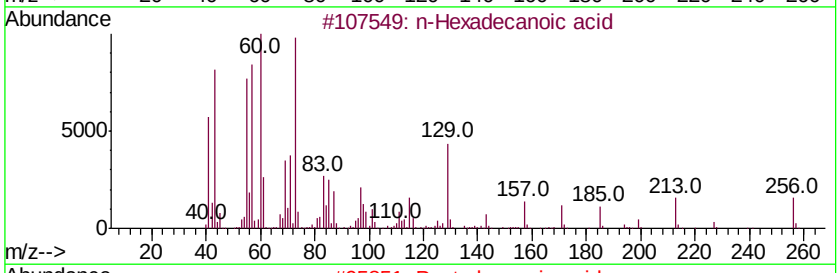
****

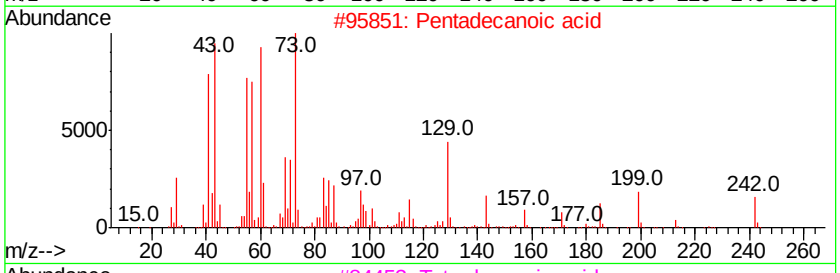
Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

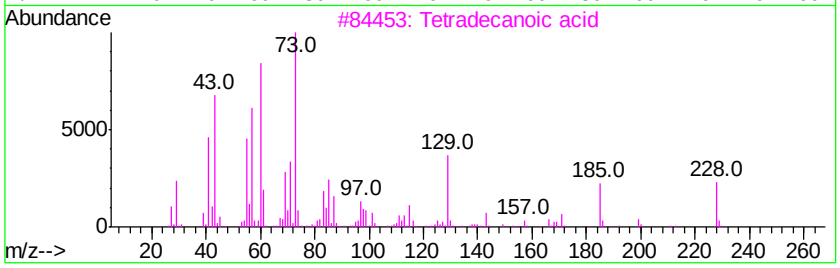
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.99	2.86 ng	72360	Phenanthrene-d10	11.49

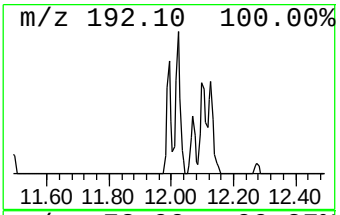
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	55
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	46
4	Tridecanoic acid	214	C13H26O2	000638-53-9	43
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	43

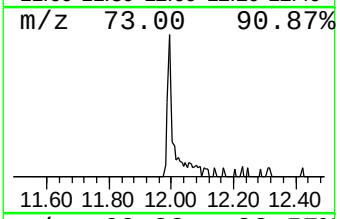


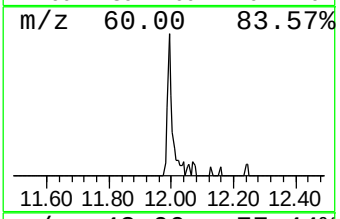


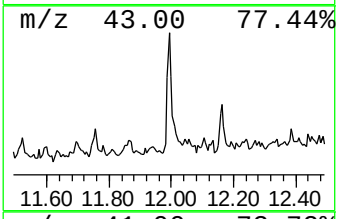


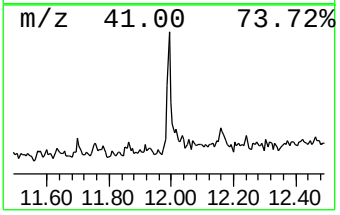












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Sample : J5769-17
Misc :
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Instrument : BNA_F
ClientSampleId : GOFFLE-RD-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

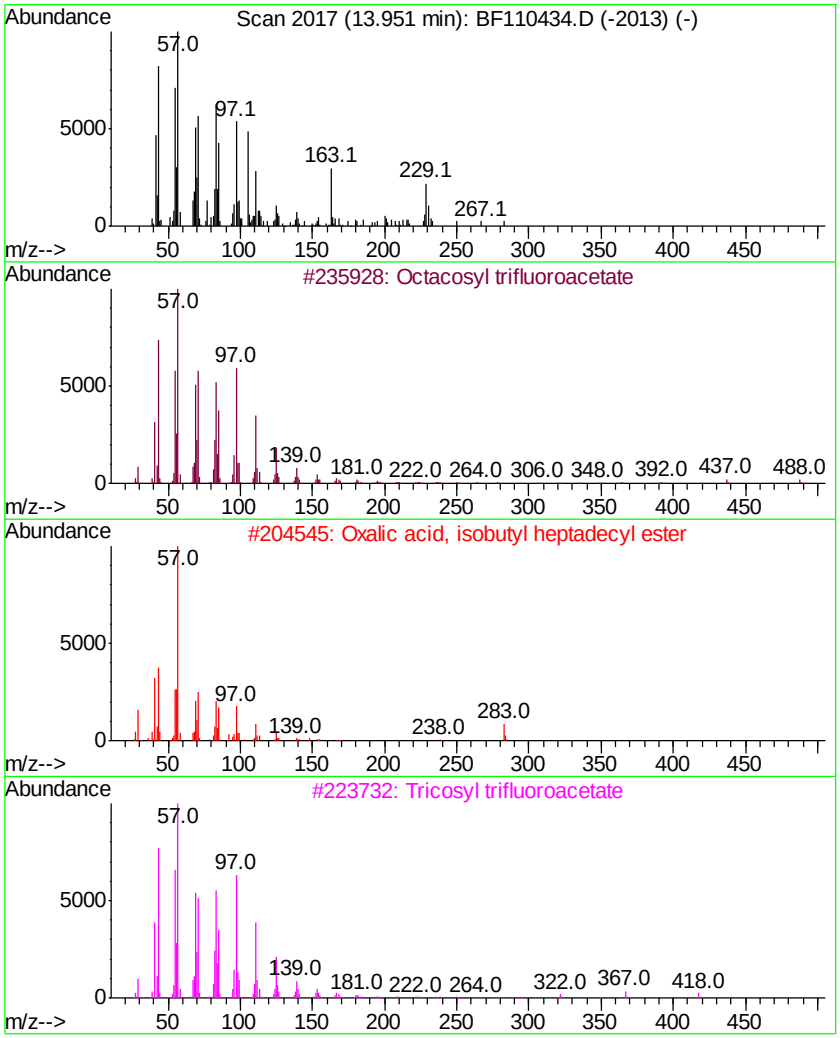
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

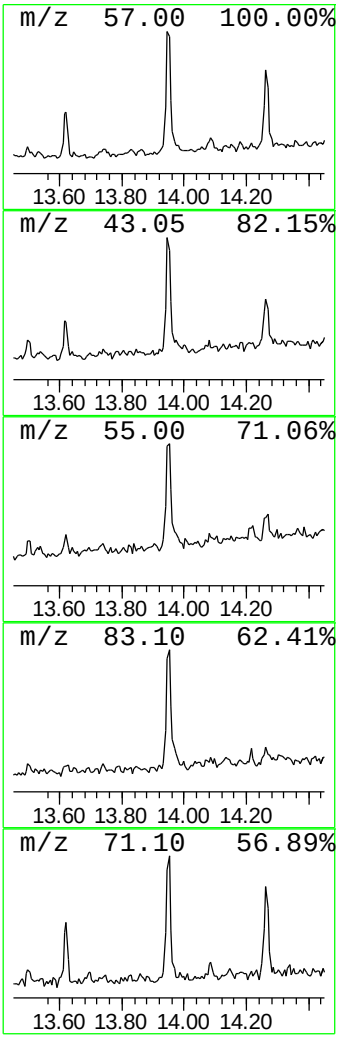
****

Peak Number 6 Octacosyl trifluoroacetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	6.05 ng	154528	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	76
2	Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	76
3	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	70
4	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	68
5	Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	68





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Data File : BF110434.D
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Sample : J5769-17
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GOFFLE-RD-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

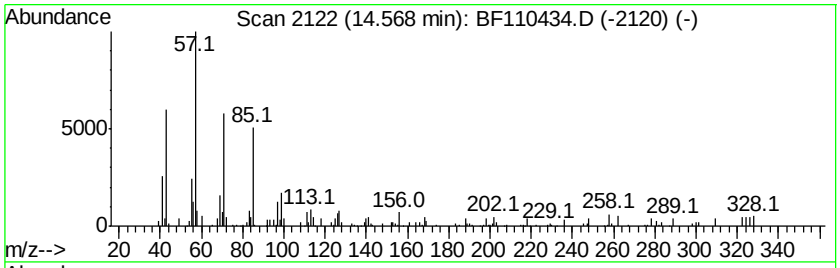
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

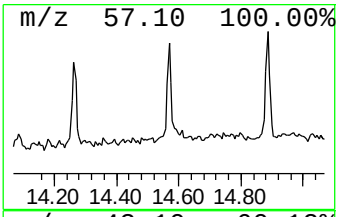
****

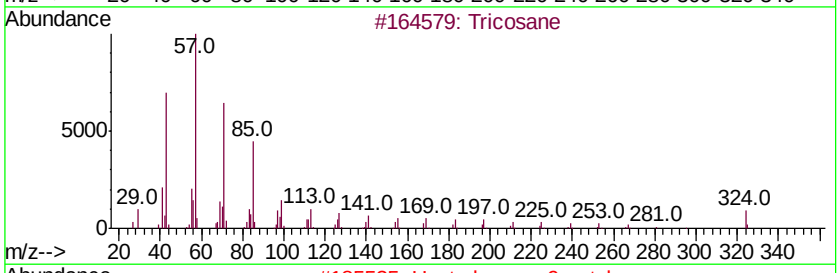
Peak Number 7 Tricosane Concentration Rank 9

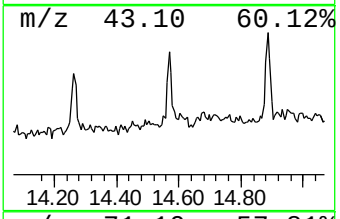
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.57	2.22 ng	56815	Chrysene-d12	14.13

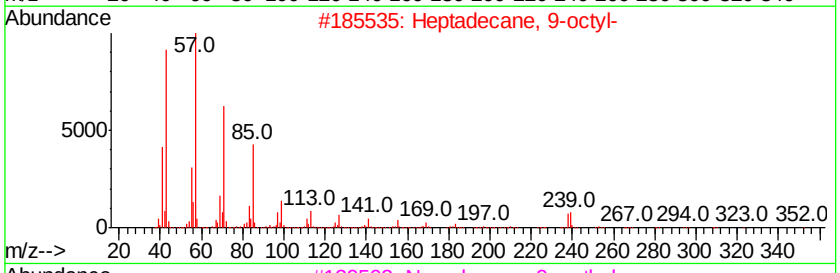
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosane	324	C23H48	000638-67-5	62
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	58
3	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	52
4	Triacontane	422	C30H62	000638-68-6	52
5	1-Iodoundecane	282	C11H23I	004282-44-4	52

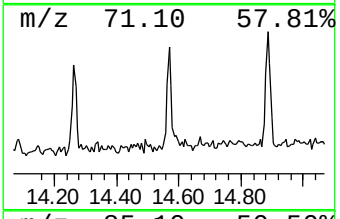


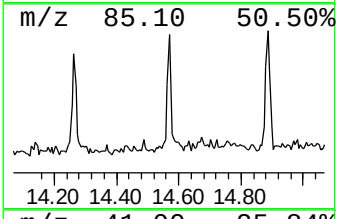


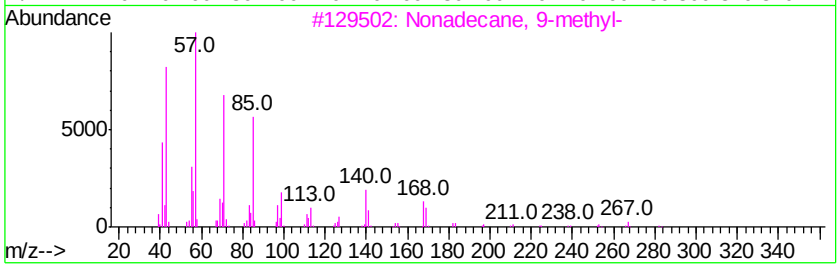


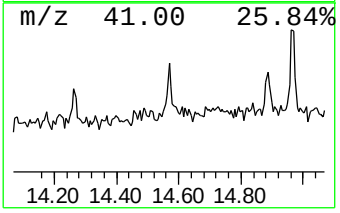












Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110218\
Data File : BF110434.D
Acq On : 3 Nov 2018 1:32
Operator : JU/SJ
Sample : J5769-17
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GOFFLE-RD-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.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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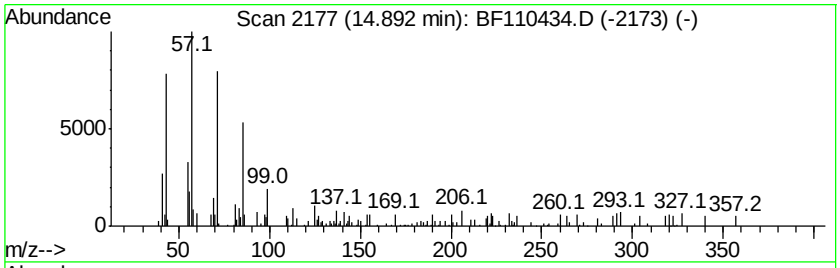
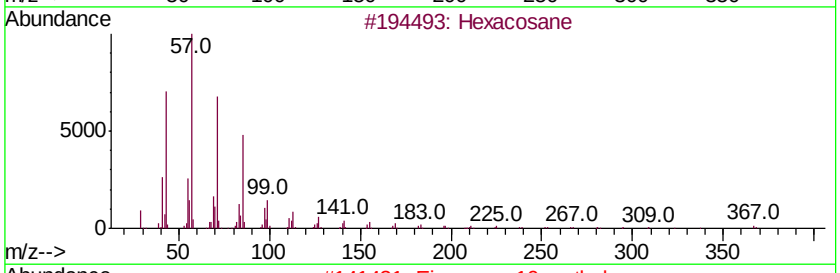
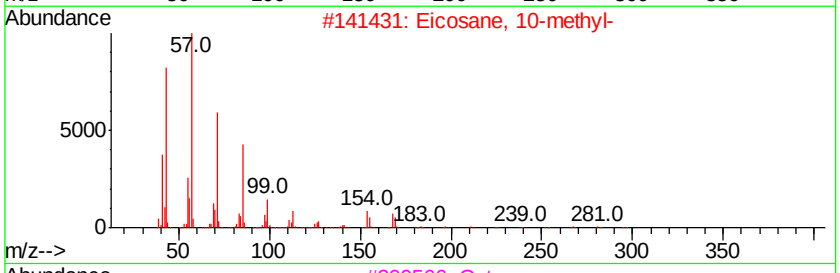
Peak Number 8 Hexacosane Concentration Rank 8

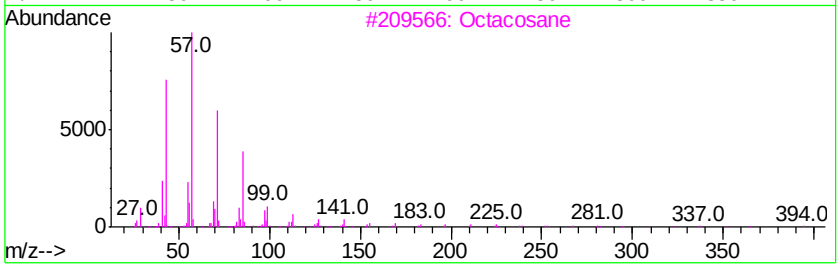
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.89	2.27 ng	58088	Chrysene-d12	14.13

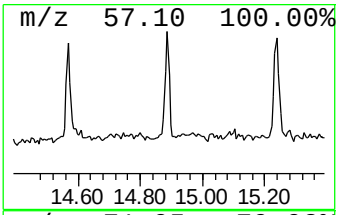
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	74
2	Eicosane, 10-methyl-	296	C21H44	054833-23-7	72
3	Octacosane	394	C28H58	000630-02-4	72
4	Heptadecane, 2-methyl-	254	C18H38	001560-89-0	64
5	Tetratetracontane	619	C44H90	007098-22-8	58

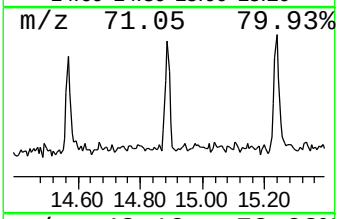


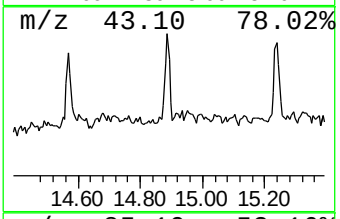


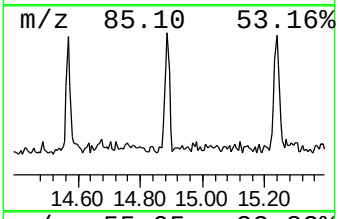


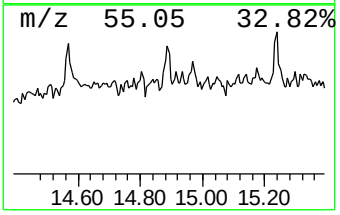












Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110218\
Data File : BF110434.D
Acq On : 3 Nov 2018 1:32
Operator : JU/SJ
Sample : J5769-17
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GOFFLE-RD-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.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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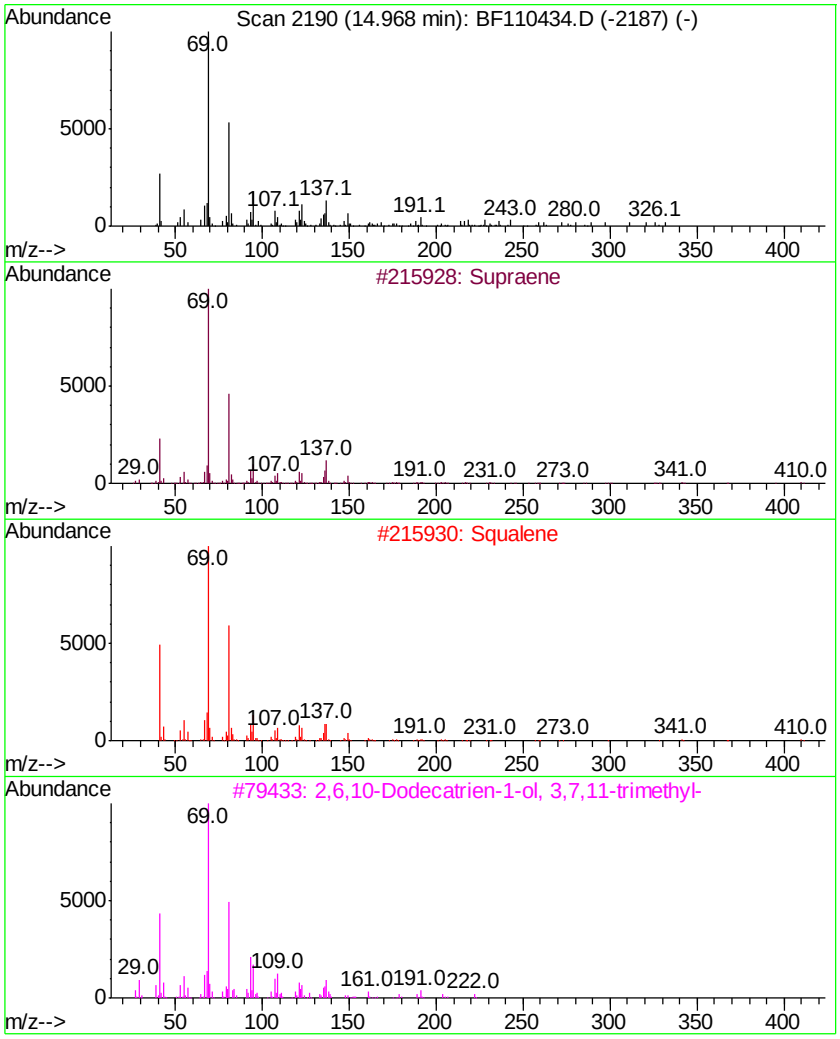
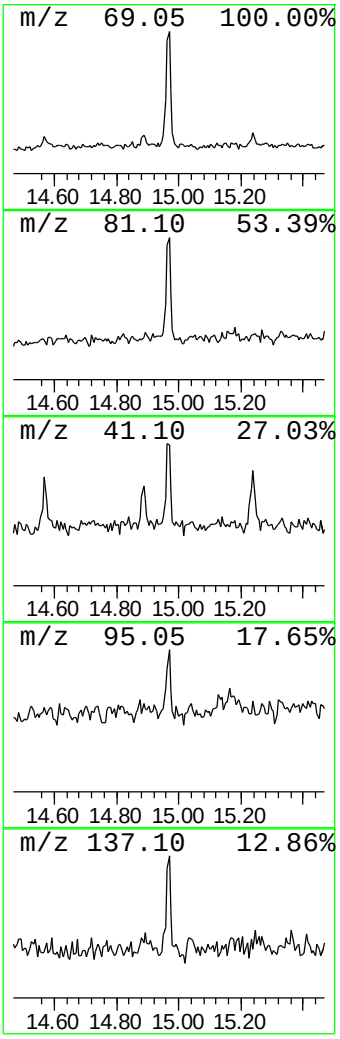
Peak Number 9 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.97	4.98 ng	80209	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	72
2	Squalene	410	C30H50	000111-02-4	72
3	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	64
4	1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	59
5	Farnesol isomer a	222	C15H26O	1000108-92-4	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF110218\
Data File : BF110434.D
Acq On : 3 Nov 2018 1:32
Operator : JU/SJ
Sample : J5769-17
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GOFFLE-RD-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.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...	2.29	18.5	ng	451588	1	6.96	487617	20.0
2-Pentanone, 4-hy...	5.20	3.0	ng	73187	1	6.96	487617	20.0
unknown6.73	6.73	75.7	ng	1844340	1	6.96	487617	20.0
n-Hexadecanoic acid	11.99	2.9	ng	72360	4	11.49	506067	20.0
Octacosyl trifluo...	13.95	6.0	ng	154528	5	14.13	511190	20.0
Tricosane	14.57	2.2	ng	56815	5	14.13	511190	20.0
Hexacosane	14.89	2.3	ng	58088	5	14.13	511190	20.0
Supraene	14.97	5.0	ng	80209	6	15.66	321941	20.0