LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021319\
Data File : BF112548.D
Acq On : 13 Feb 2019 19:35
Operator : JU/SJ
Sample : K1458-08 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-5

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	5.040	499	502	512	rBV	64600	82386	6.55%	0.535%
2	5.469	572	575	594	rBV	909621	1067842	84.87%	6.936%
3	5.604	594	598	603	rVB3	17042	25584	2.03%	0.166%
4	5.846	634	639	645	rBB3	12341	22278	1.77%	0.145%
5	5.987	657	663	668	rVB2	13981	17713	1.41%	0.115%
6	6.087	674	680	682	rBV3	15629	23306	1.85%	0.151%
7	6.269	705	711	714	rBV3	12604	14760	1.17%	0.096%
8	6.363	724	727	733	rBV2	41505	48508	3.86%	0.315%
9	6.487	744	748	758	rBV	986214	1168336	92.85%	7.589%
10	6.557	758	760	763	rVV4	32744	36098	2.87%	0.234%
11	6.610	766	769	777	rVB	1293257	1228106	97.60%	7.977%
12	6.834	804	807	814	rVB	759093	657135	52.23%	4.268%
13	6.993	830	834	843	rVB	1088360	952009	75.66%	6.184%
14	7.104	850	853	858	rVB2	27791	30774	2.45%	0.200%
15	7.228	868	874	876	rBV4	20422	21880	1.74%	0.142%
16	7.357	891	896	900	rBV4	20097	38974	3.10%	0.253%
17	7.398	900	903	912	rVV	698982	699784	55.61%	4.545%
18	7.475	912	916	920	rVB3	29753	44394	3.53%	0.288%
19	7.534	920	926	929	rBV4	11455	26567	2.11%	0.173%
20	7.610	937	939	942	rBV	35925	27236	2.16%	0.177%
21	7.640	942	944	947	rVV3	29421	22984	1.83%	0.149%
22	7.710	951	956	958	rBV3	21575	27827	2.21%	0.181%
23	7.757	961	964	968	rVB3	39403	41680	3.31%	0.271%
24	7.857	979	981	983	rBV3	13442	14000	1.11%	0.091%
25	7.934	991	994	1000	rVB7	15026	21975	1.75%	0.143%
26	7.987	1000	1003	1006	rBV3	16293	22363	1.78%	0.145%
27	8.022	1006	1009	1013	rBV6	12243	16008	1.27%	0.104%
28	8.057	1013	1015	1019	rBV4	23314	28816	2.29%	0.187%
29	8.116	1022	1025	1031	rVV	793959	822408	65.36%	5.342%
30	8.175	1031	1035	1037	rVV3	63320	77947	6.19%	0.506%
31	8.198	1037	1039	1042	rVV3	20663	20846	1.66%	0.135%
32	8.322	1057	1060	1062	rBV	30722	26584	2.11%	0.173%
33	8.345	1062	1064	1067	rBV	17578	14649	1.16%	0.095%
34	8.404	1067	1074	1079	rBV5	51322	87187	6.93%	0.566%

LSC Area Percent Report

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Operator : JU/SJ
Sample : K1458-08 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-5

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	8.463	1081	1084	1087	rBV4	16725	17352	1.38%	0.113%
36	8.498	1087	1090	1093	rVB5	19017	21907	1.74%	0.142%
37	8.534	1093	1096	1098	rBV	70250	62503	4.97%	0.406%
38	8.557	1098	1100	1101	rBV2	26894	19913	1.58%	0.129%
39	8.575	1101	1103	1107	rVB4	40841	41514	3.30%	0.270%
40	8.622	1108	1111	1113	rBV2	31270	23780	1.89%	0.154%
41	8.657	1113	1117	1119	rBV3	34963	35950	2.86%	0.234%
42	8.704	1122	1125	1129	rBV4	18019	23237	1.85%	0.151%
43	8.745	1129	1132	1134	rBV4	17433	21639	1.72%	0.141%
44	8.798	1139	1141	1146	rVB4	42069	46950	3.73%	0.305%
45	8.863	1149	1152	1154	rVB2	35129	29400	2.34%	0.191%
46	8.892	1154	1157	1160	rBV5	24317	32132	2.55%	0.209%
47	8.939	1163	1165	1167	rBV3	30414	25625	2.04%	0.166%
48	9.022	1177	1179	1183	rVB3	32673	30345	2.41%	0.197%
49	9.063	1183	1186	1191	rBV5	23688	45868	3.65%	0.298%
50	9.110	1191	1194	1196	rVB3	40562	31860	2.53%	0.207%
51	9.134	1196	1198	1204	rBV3	102855	101982	8.10%	0.662%
52	9.192	1204	1208	1213	rBV	1335247	1258265	100.00%	8.173%
53	9.269	1218	1221	1224	rBV3	82575	92368	7.34%	0.600%
54	9.316	1226	1229	1231	rBV3	26893	34186	2.72%	0.222%
55	9.463	1251	1254	1258	rBV4	37201	36755	2.92%	0.239%
56	9.534	1263	1266	1271	rVB4	47874	78623	6.25%	0.511%
57	9.581	1271	1274	1278	rBV2	222900	273521	21.74%	1.777%
58	9.739	1298	1301	1303	rBV3	68602	70563	5.61%	0.458%
59	9.781	1306	1308	1313	rVV2	106733	95389	7.58%	0.620%
60	9.875	1317	1324	1334	rVV2	897895	974011	77.41%	6.327%
61	9.981	1338	1342	1346	rBV4	33481	46479	3.69%	0.302%
62	10.028	1346	1350	1353	rVV5	21284	31623	2.51%	0.205%
63	10.081	1357	1359	1363	rVB3	33249	38472	3.06%	0.250%
64	10.122	1363	1366	1369	rBV3	48266	48694	3.87%	0.316%
65	10.192	1374	1378	1381	rBV3	52992	64720	5.14%	0.420%
66	10.281	1389	1393	1395	rBV4	47317	55192	4.39%	0.359%
67	10.328	1399	1401	1403	rBV2	14582	14158	1.13%	0.092%
68	10.516	1430	1433	1440	rVB2	44611	62938	5.00%	0.409%
69	10.569	1440	1442	1447	rVB4	19571	22846	1.82%	0.148%
70	10.669	1456	1459	1469	rBV	605227	655231	52.07%	4.256%
71	10.786	1473	1479	1486	rVB2	80446	111168	8.84%	0.722%

LSC Area Percent Report

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Sample : K1458-08 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-5

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
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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	10.998	1513	1515	1520	rVB3	19105	20074	1.60%	0.130%
73	11.245	1554	1557	1564	rVB2	46712	56324	4.48%	0.366%
74	11.363	1574	1577	1591	rBV	698606	768747	61.10%	4.993%
75	11.698	1631	1634	1638	rVB5	12304	15716	1.25%	0.102%
76	11.880	1662	1665	1673	rBV3	92845	117632	9.35%	0.764%
77	12.422	1754	1757	1758	rBV	20244	19514	1.55%	0.127%
78	12.586	1782	1785	1786	rBV3	19708	20715	1.65%	0.135%
79	12.616	1787	1790	1794	rVV	62904	67306	5.35%	0.437%
80	12.669	1797	1799	1803	rBV4	35369	53481	4.25%	0.347%
81	12.945	1842	1846	1852	rBV	1108283	939400	74.66%	6.102%
82	13.833	1994	1997	2005	rBV2	137673	192762	15.32%	1.252%
83	14.016	2025	2028	2032	rBV	706732	611480	48.60%	3.972%
84	15.504	2278	2281	2285	rVB	304628	355894	28.28%	2.312%

Sum of corrected areas: 15395148

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021319\
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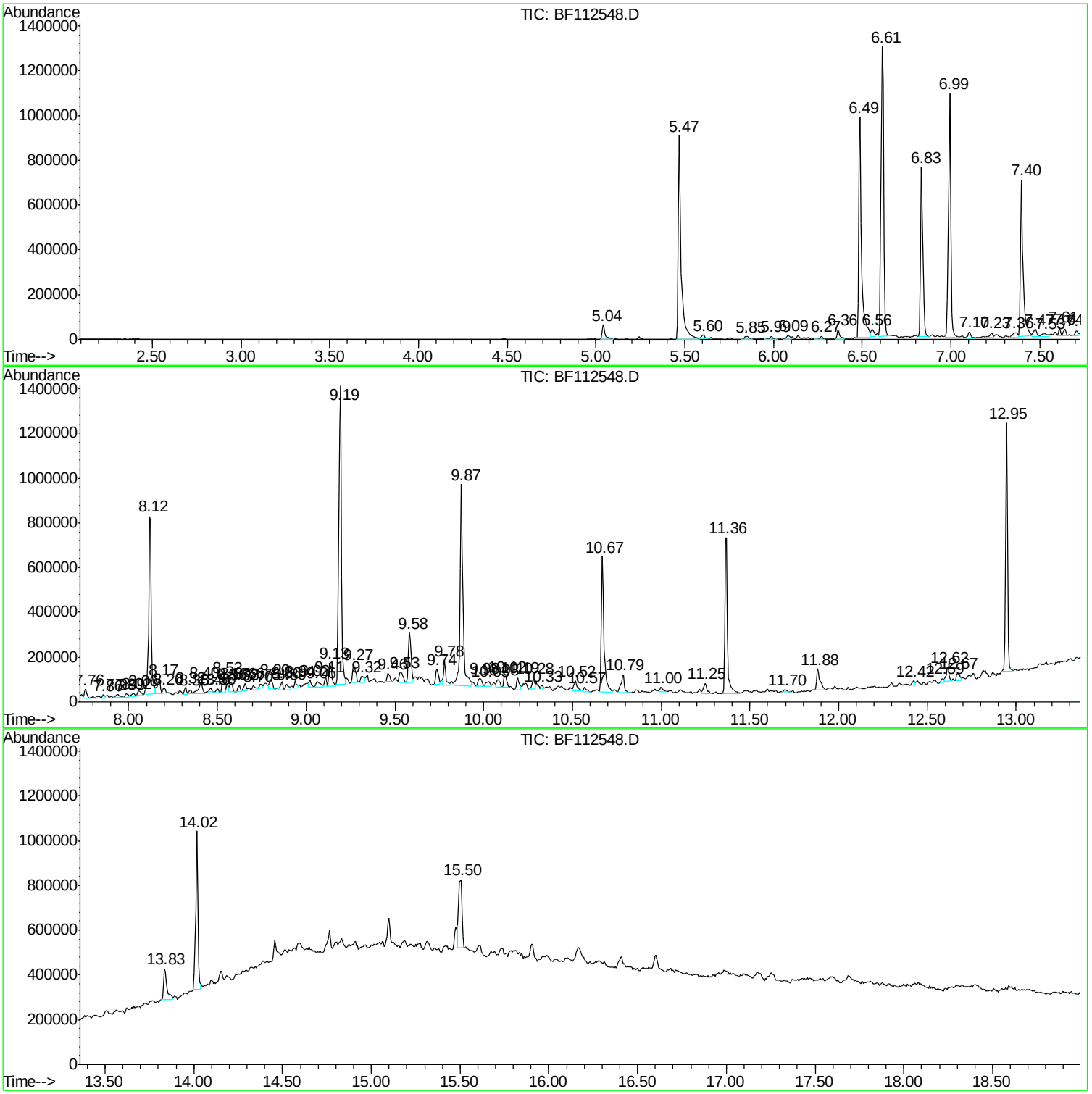
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-5

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

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021319\
Data File : BF112548.D
Acq On : 13 Feb 2019 19:35
Operator : JU/SJ
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Misc :
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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

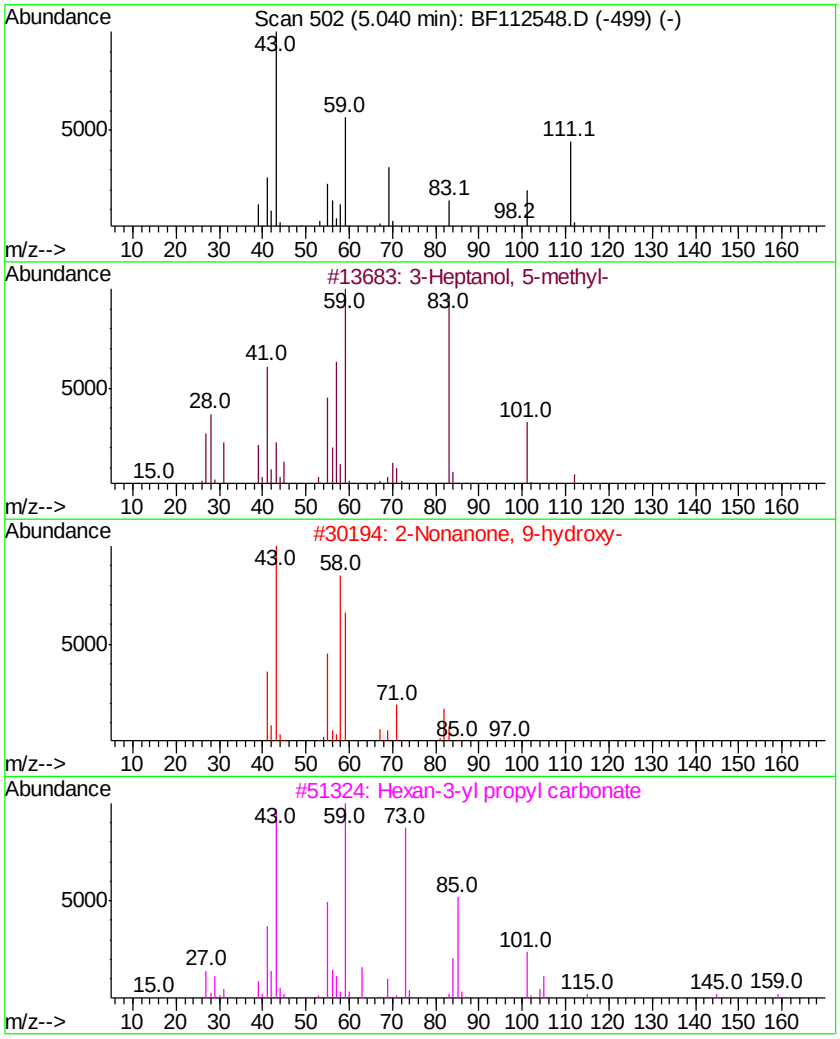
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

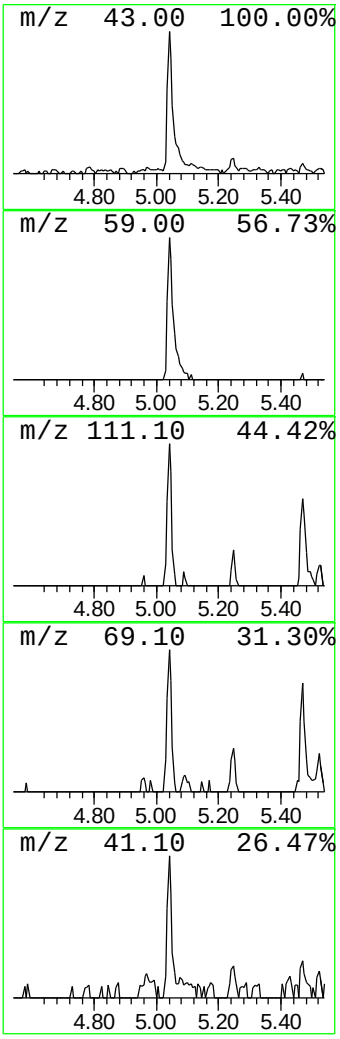
****

Peak Number 1 unknown5.04 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	2.51 ng	82386	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Heptanol, 5-methyl-	130	C8H18O	018720-65-5	32
2	2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	23
3	Hexan-3-yl propyl carbonate	188	C10H20O3	1000372-82-0	17
4	3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	16
5	5-Ethyl-3-methylhept-1-en-4-ol	156	C10H20O	286424-80-4	10





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021319\
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Sample : K1458-08 2X
Misc :
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Instrument : BNA_F
ClientSampleId : SB-5

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

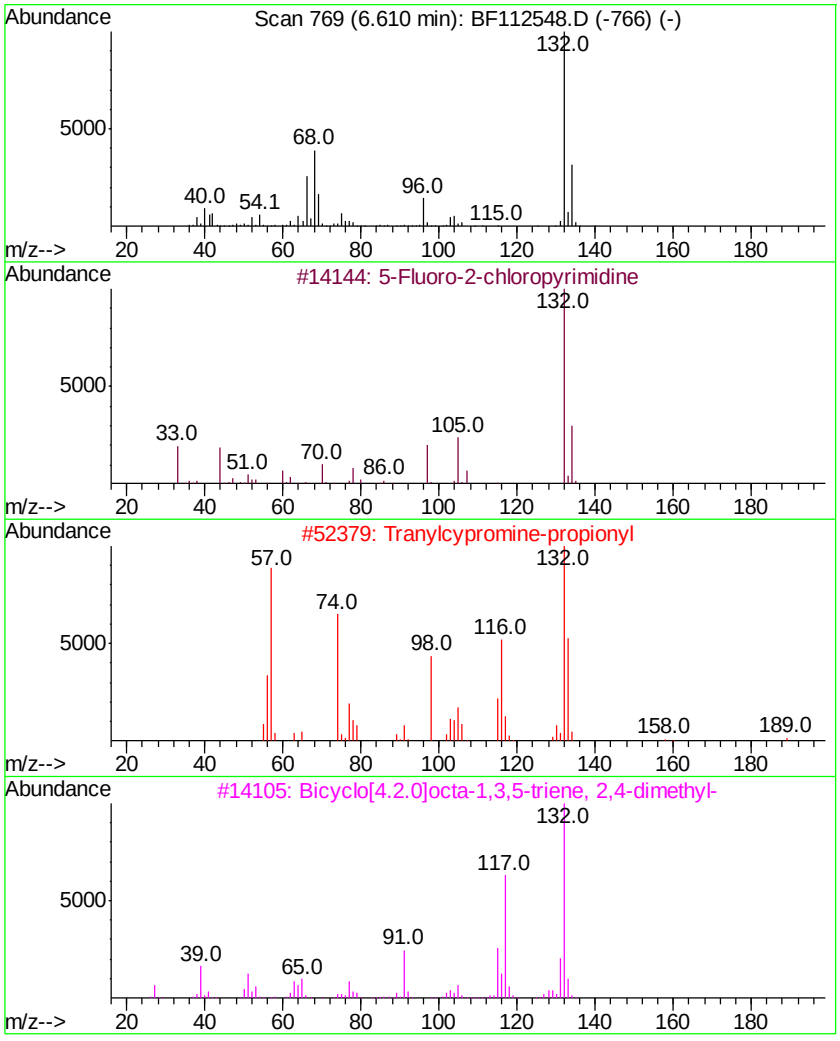
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

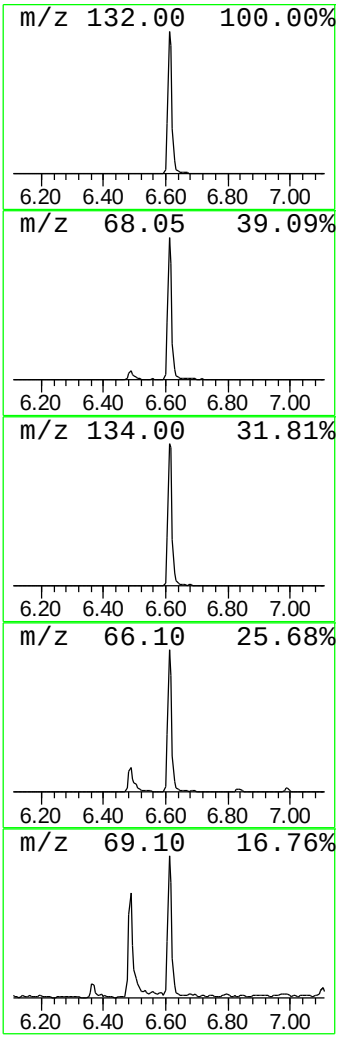
****

Peak Number 2 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	37.38 ng	1228110	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





Library Search Compound Report

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
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TIC Library : C:\DATABASE\NIST11.L
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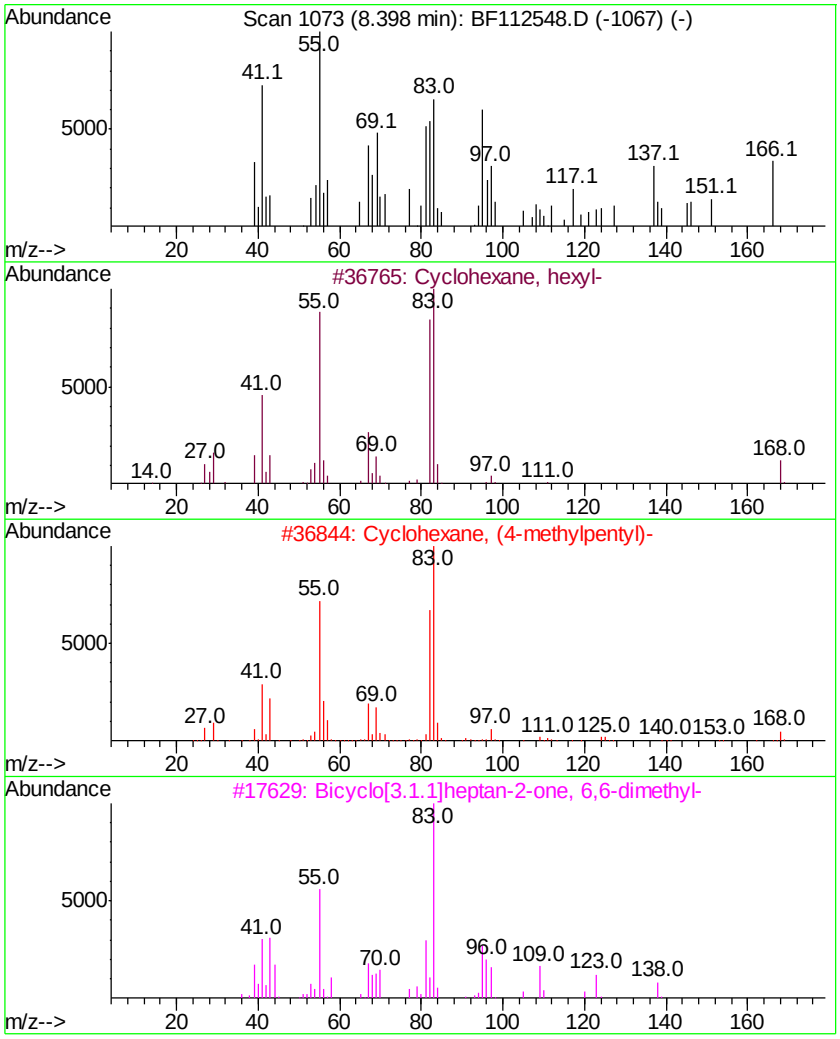
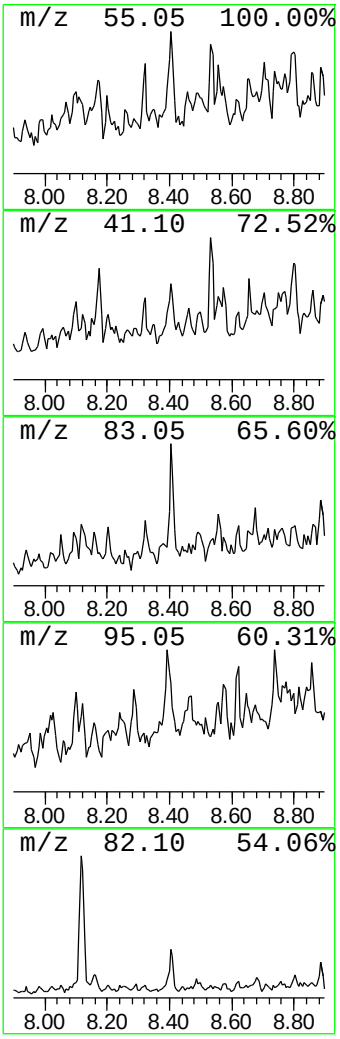
Peak Number 4 unknown8.40 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.40	2.12 ng	87187	Naphthalene-d8	8.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, hexyl-	168	C12H24	004292-75-5	46
2	Cyclohexane, (4-methylpentyl)-	168	C12H24	061142-20-9	45
3	Bicyclo[3.1.1]heptan-2-one, 6,6-...	138	C9H14O	024903-95-5	43
4	Cyclododecene	166	C12H22	001501-82-2	41
5	Cyclohexane, 2-propenyl-	124	C9H16	002114-42-3	38





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TIC Library : C:\DATABASE\NIST11.L
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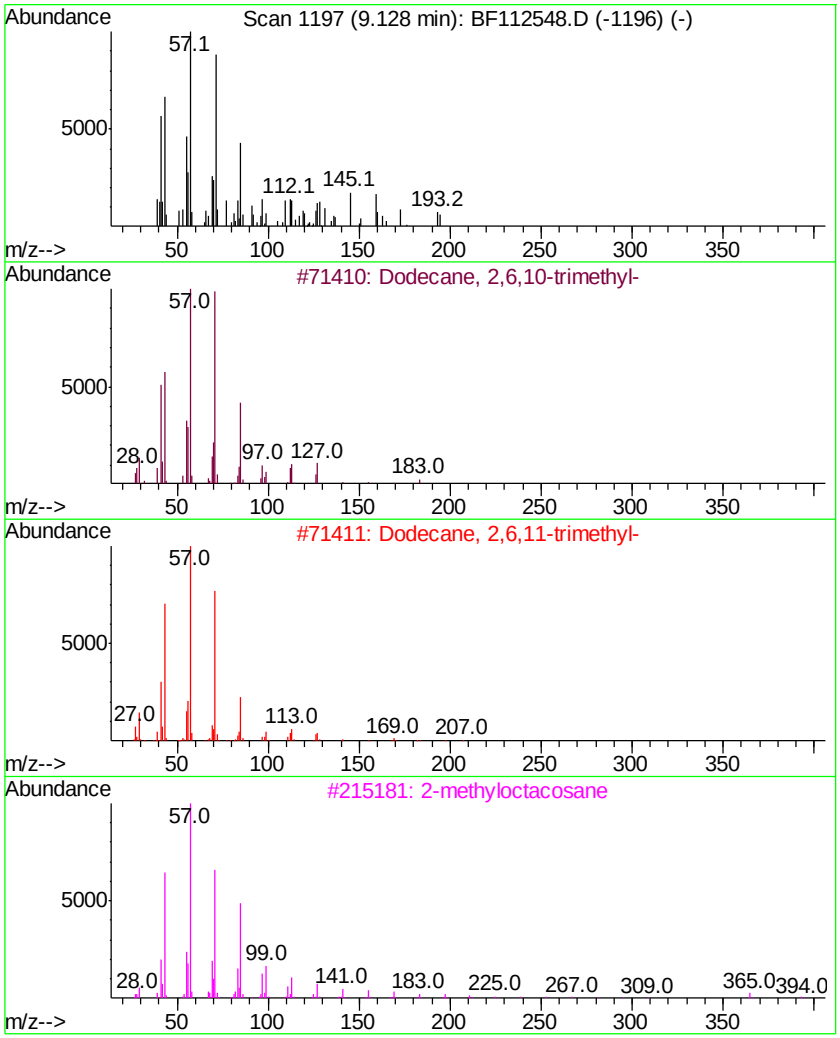
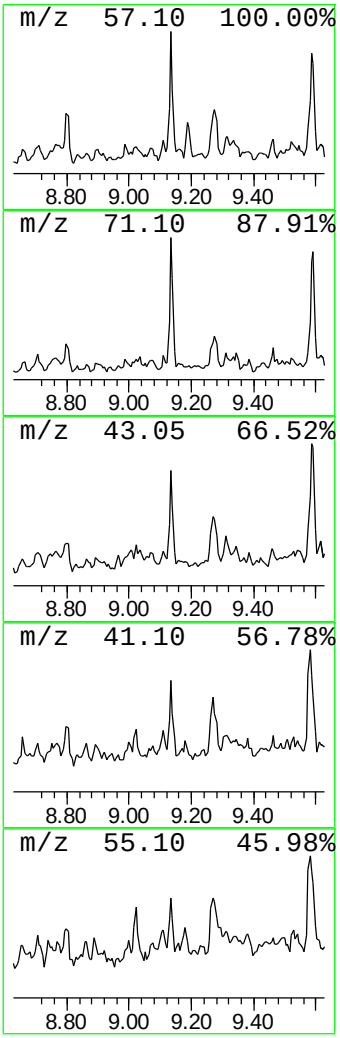
Peak Number 5 Dodecane, 2,6,10-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.13	2.09 ng	101982	Acenaphthene-d10	9.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	68
2	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	59
3	2-methyloctacosane	408	C29H60	1000376-72-8	53
4	Heptadecane	240	C17H36	000629-78-7	52
5	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	52





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Misc :
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Instrument : BNA_F
ClientSampleId : SB-5

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

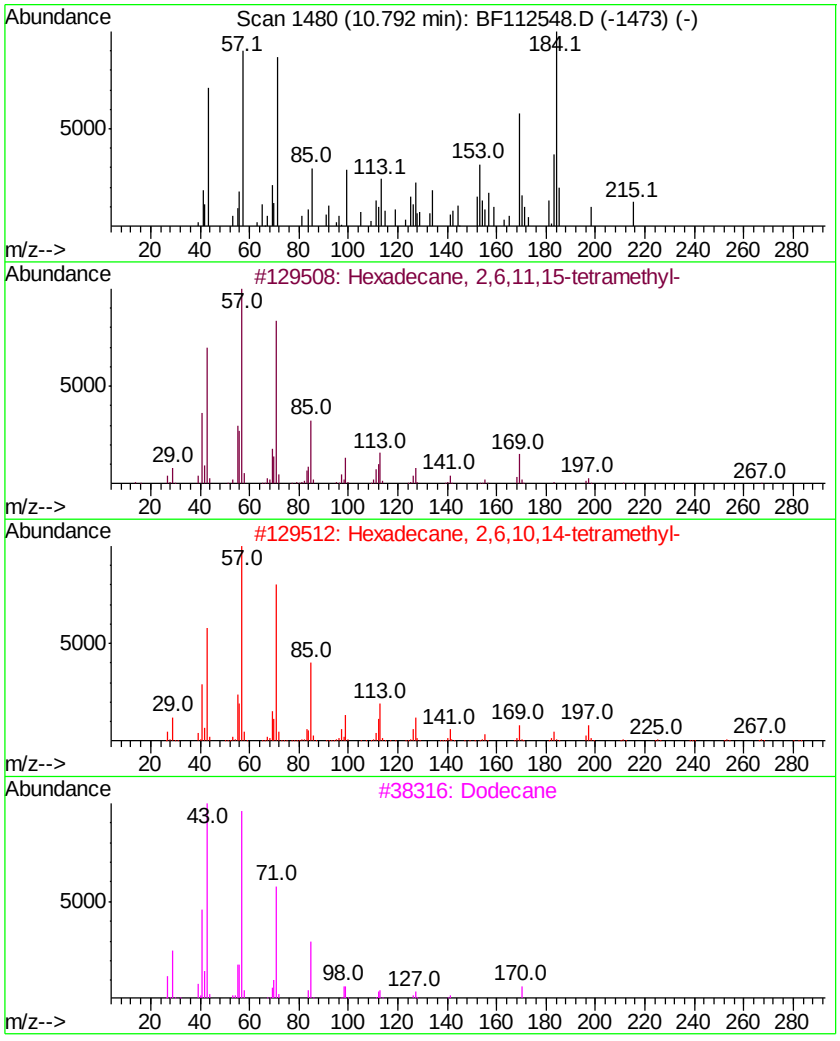
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

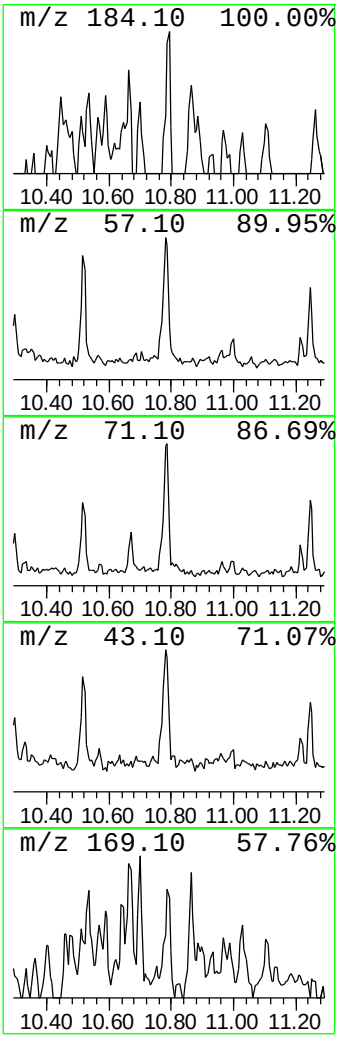
****

Peak Number 6 Hexadecane, 2,6,11,15-tetra... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.79	2.89 ng	111168	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2,6,11,15-tetramethyl-	282	C20H42	000504-44-9	72
2	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	64
3	Dodecane	170	C12H26	000112-40-3	53
4	Hexadecane, 2,6,10-trimethyl-	268	C19H40	055000-52-7	47
5	Sulfurous acid, 2-ethylhexyl tet...	390	C22H46O3S	1000309-19-7	43





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Misc :
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Instrument : BNA_F
ClientSampleId : SB-5

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

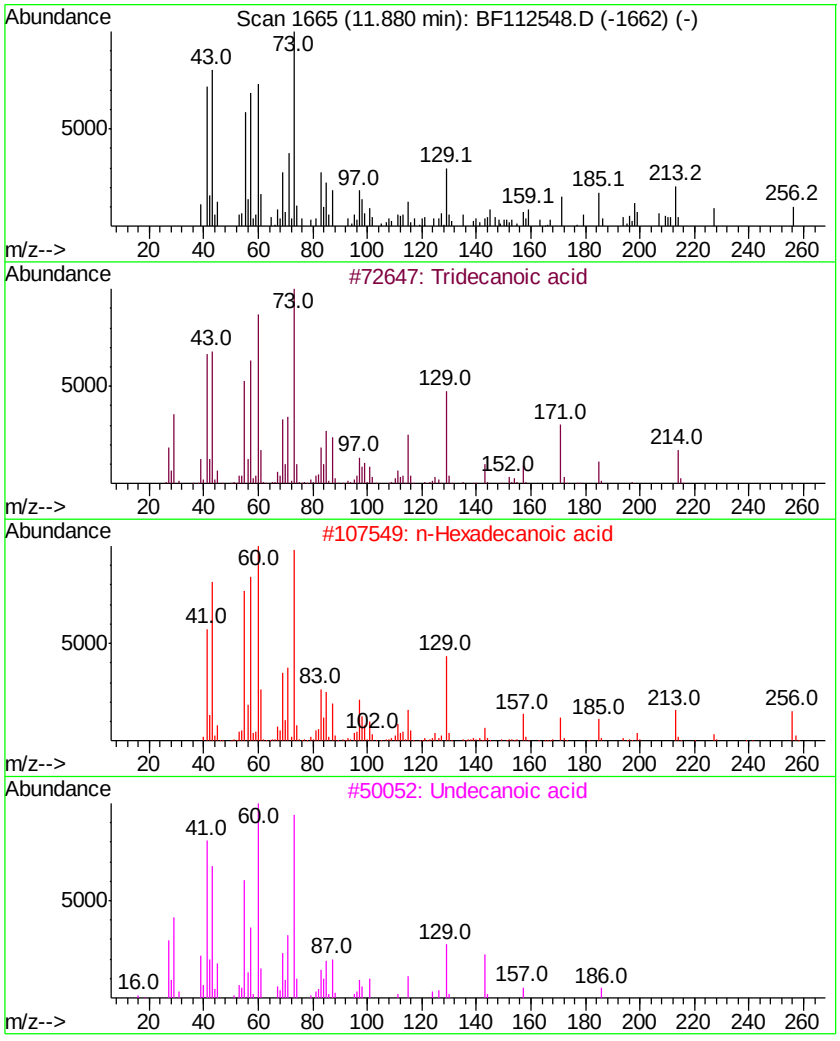
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

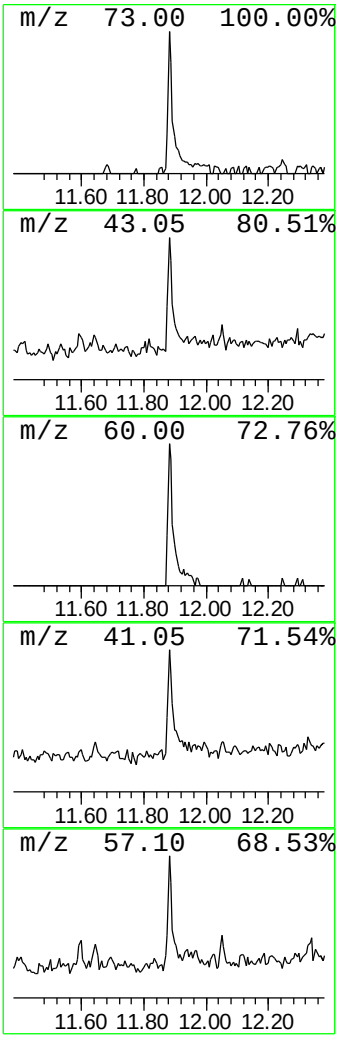
****

Peak Number 7 Tridecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.88	3.06 ng	117632	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	90
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
3	Undecanoic acid	186	C11H22O2	000112-37-8	70
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	53
5	n-Decanoic acid	172	C10H20O2	000334-48-5	38





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021319\
Data File : BF112548.D
Acq On : 13 Feb 2019 19:35
Operator : JU/SJ
Sample : K1458-08 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-5

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

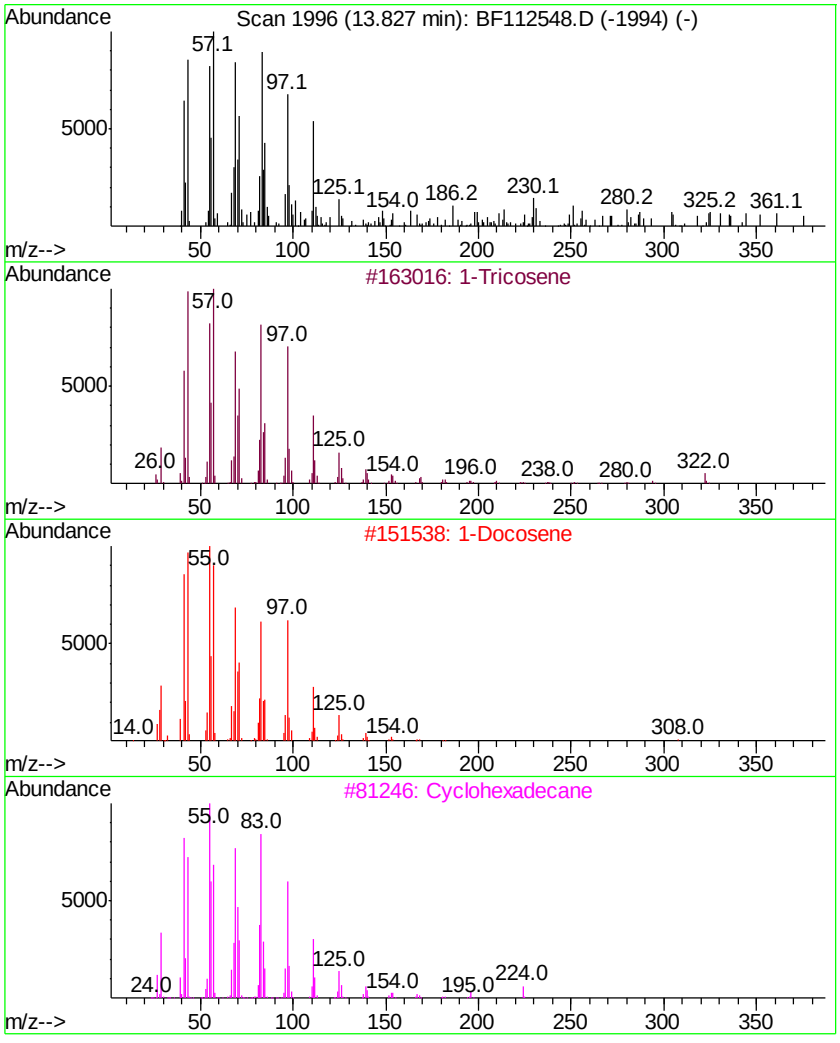
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

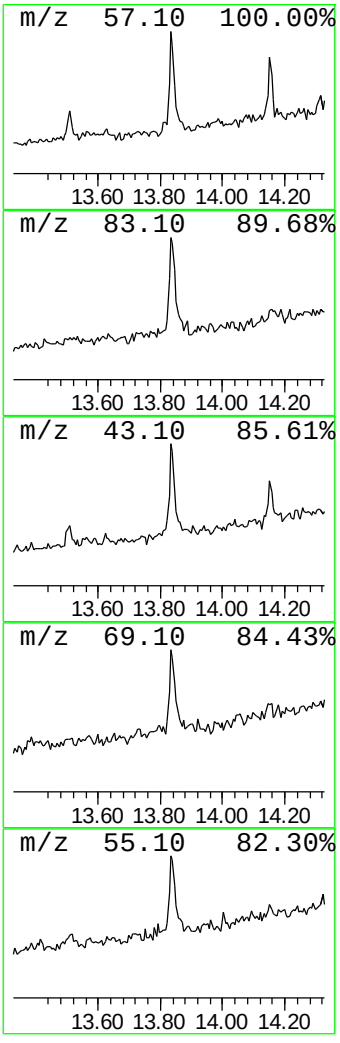
****

Peak Number 8 1-Tricosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	6.30 ng	192762	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tricosene	322	C23H46	018835-32-0	95
2	1-Docosene	308	C22H44	001599-67-3	93
3	Cyclohexadecane	224	C16H32	000295-65-8	93
4	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	93
5	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF021319\
Data File : BF112548.D
Acq On : 13 Feb 2019 19:35
Operator : JU/SJ
Sample : K1458-08 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-5

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
unknown5.04	5.04	2.5	ng	82386	1	6.83	657135	20.0
unknown6.61	6.61	37.4	ng	1228110	1	6.83	657135	20.0
unknown8.40	8.40	2.1	ng	87187	2	8.12	822408	20.0
Dodecane, 2,6,10-...	9.13	2.1	ng	101982	3	9.87	974011	20.0
Hexadecane, 2,6,1...	10.79	2.9	ng	111168	4	11.36	768747	20.0
Tridecanoic acid	11.88	3.1	ng	117632	4	11.36	768747	20.0
1-Tricosene	13.83	6.3	ng	192762	5	14.02	611480	20.0