LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012419\
Data File : BF112215.D
Acq On : 24 Jan 2019 18:10
Operator : JU/SJ
Sample : K1223-03 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TS-O

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-BF011619.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	2.657	91	97	106	rBV	23492	40618	1.98%	0.133%
2	5.057	502	505	512	rBV	60734	63930	3.12%	0.209%
3	5.487	574	578	591	rBV	1405882	1345678	65.65%	4.409%
4	6.498	746	750	765	rBV	2056499	1882966	91.86%	6.170%
5	6.628	769	772	780	rVB	2346251	1985679	96.87%	6.507%
6	6.851	807	810	819	rBV	1497252	1374496	67.06%	4.504%
7	7.010	833	837	844	rBV	1857092	1500923	73.22%	4.918%
8	7.410	901	905	916	rVB	1208277	1141968	55.71%	3.742%
9	8.139	1025	1029	1032	rBV	2013474	1745028	85.13%	5.718%
10	9.039	1179	1182	1186	rVB2	23112	24920	1.22%	0.082%
11	9.210	1207	1211	1221	rBV	2379917	2018252	98.46%	6.613%
12	9.292	1221	1225	1227	rVB3	26024	30781	1.50%	0.101%
13	9.363	1233	1237	1242	rVB5	36325	60843	2.97%	0.199%
14	9.469	1253	1255	1262	rBV6	16765	23482	1.15%	0.077%
15	9.528	1262	1265	1266	rBV2	52358	41963	2.05%	0.138%
16	9.551	1266	1269	1272	rVV	379372	303203	14.79%	0.994%
17	9.604	1275	1278	1282	rVB	196206	191997	9.37%	0.629%
18	9.651	1282	1286	1288	rBV	95100	82335	4.02%	0.270%
19	9.804	1310	1312	1314	rBV3	40444	32118	1.57%	0.105%
20	9.892	1321	1327	1331	rBV2	2182215	2049783	100.00%	6.717%
21	9.922	1331	1332	1335	rVV	146239	95435	4.66%	0.313%
22	9.963	1337	1339	1342	rVB2	44713	43066	2.10%	0.141%
23	10.016	1342	1348	1352	rBV3	184119	273843	13.36%	0.897%
24	10.098	1358	1362	1365	rVB2	70253	71847	3.51%	0.235%
25	10.186	1374	1377	1379	rBV	65422	49012	2.39%	0.161%
26	10.316	1395	1399	1402	rVB4	27924	40282	1.97%	0.132%
27	10.439	1417	1420	1425	rBV	79822	68595	3.35%	0.225%
28	10.486	1425	1428	1430	rBV3	28831	36281	1.77%	0.119%
29	10.533	1433	1436	1439	rBV3	96290	81268	3.96%	0.266%
30	10.563	1439	1441	1444	rVB	117649	89360	4.36%	0.293%
31	10.598	1444	1447	1448	rBV2	31821	27649	1.35%	0.091%
32	10.616	1448	1450	1453	rVB2	39221	32696	1.60%	0.107%
33	10.657	1453	1457	1458	rBV4	36730	51586	2.52%	0.169%
34	10.680	1458	1461	1466	rBV	1228996	1193204	58.21%	3.910%

LSC Area Percent Report

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Sample : K1223-03 2X
Misc :
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Instrument : BNA_F
ClientSampleId : TS-O

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-BF011619.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	10.804	1478	1482	1489	rVB4	96563	151344	7.38%	0.496%
36	10.863	1489	1492	1494	rBV3	22963	30533	1.49%	0.100%
37	10.922	1499	1502	1506	rBV5	27592	37560	1.83%	0.123%
38	10.986	1511	1513	1517	rVB4	25785	23762	1.16%	0.078%
39	11.045	1520	1523	1524	rBV3	24877	26835	1.31%	0.088%
40	11.098	1529	1532	1534	rVV3	48466	56173	2.74%	0.184%
41	11.116	1534	1535	1540	rVV4	46272	54800	2.67%	0.180%
42	11.186	1544	1547	1549	rVB	42461	42231	2.06%	0.138%
43	11.239	1554	1556	1558	rVV2	39203	41891	2.04%	0.137%
44	11.275	1560	1562	1567	rVB2	50591	60858	2.97%	0.199%
45	11.380	1576	1580	1582	rBV	1919707	1674844	81.71%	5.488%
46	11.404	1582	1584	1587	rVV	710899	588536	28.71%	1.928%
47	11.427	1587	1588	1590	rVV	160719	105855	5.16%	0.347%
48	11.457	1590	1593	1596	rVV	185104	165235	8.06%	0.541%
49	11.486	1596	1598	1600	rVV2	38655	37288	1.82%	0.122%
50	11.516	1600	1603	1606	rVB	108408	102020	4.98%	0.334%
51	11.592	1613	1616	1618	rBV2	46779	54217	2.65%	0.178%
52	11.722	1635	1638	1641	rBV	110532	111553	5.44%	0.366%
53	11.763	1643	1645	1648	rVB	56383	48576	2.37%	0.159%
54	11.869	1659	1663	1667	rBV2	254648	323940	15.80%	1.061%
55	11.904	1667	1669	1677	rVV2	422657	488279	23.82%	1.600%
56	11.992	1681	1684	1687	rBV	95448	107392	5.24%	0.352%
57	12.074	1695	1698	1700	rBV	138095	104951	5.12%	0.344%
58	12.263	1728	1730	1734	rVB5	65652	58645	2.86%	0.192%
59	12.304	1734	1737	1739	rBV4	63046	78551	3.83%	0.257%
60	12.357	1744	1746	1748	rBV2	57495	44286	2.16%	0.145%
61	12.445	1755	1761	1764	rBV3	100862	217133	10.59%	0.711%
62	12.516	1770	1773	1778	rBV	704714	648692	31.65%	2.126%
63	12.598	1783	1787	1792	rBV	765085	844901	41.22%	2.769%
64	12.686	1800	1802	1806	rBV5	71795	76353	3.72%	0.250%
65	12.827	1820	1826	1832	rVV	638631	703506	34.32%	2.305%
66	12.874	1832	1834	1838	rVB2	82829	92402	4.51%	0.303%
67	12.963	1845	1849	1852	rBV	1514617	1316170	64.21%	4.313%
68	13.398	1920	1923	1926	rVB3	235697	230957	11.27%	0.757%
69	13.463	1932	1934	1936	rBV	116593	88773	4.33%	0.291%
70	13.851	1998	2000	2007	rVB2	286199	347255	16.94%	1.138%
71	14.027	2025	2030	2032	rBV2	1460189	1575504	76.86%	5.163%

LSC Area Percent Report

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Sample : K1223-03 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TS-O

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

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Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	14.051	2032	2034	2037	rVB	255920	202201	9.86%	0.663%
73	15.127	2214	2217	2219	rBV	314956	323157	15.77%	1.059%
74	15.504	2277	2281	2291	rBV	834057	1135975	55.42%	3.722%

Sum of corrected areas: 30518221

LSC Report - Integrated Chromatogram

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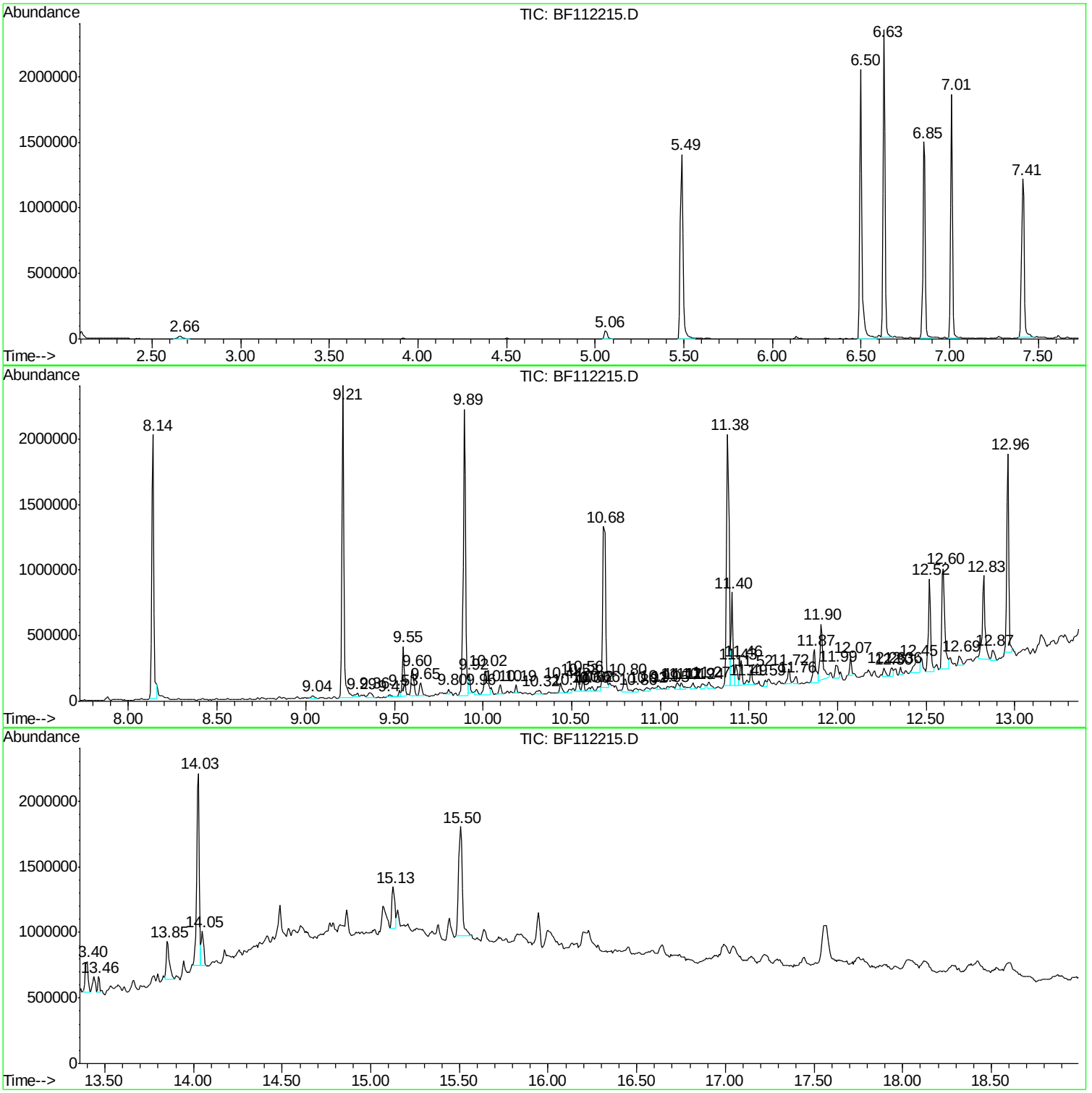
Sample : K1223-03 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TS-O

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.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\BF012419\
Data File : BF112215.D
Acq On : 24 Jan 2019 18:10
Operator : JU/SJ
Sample : K1223-03 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TS-O

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

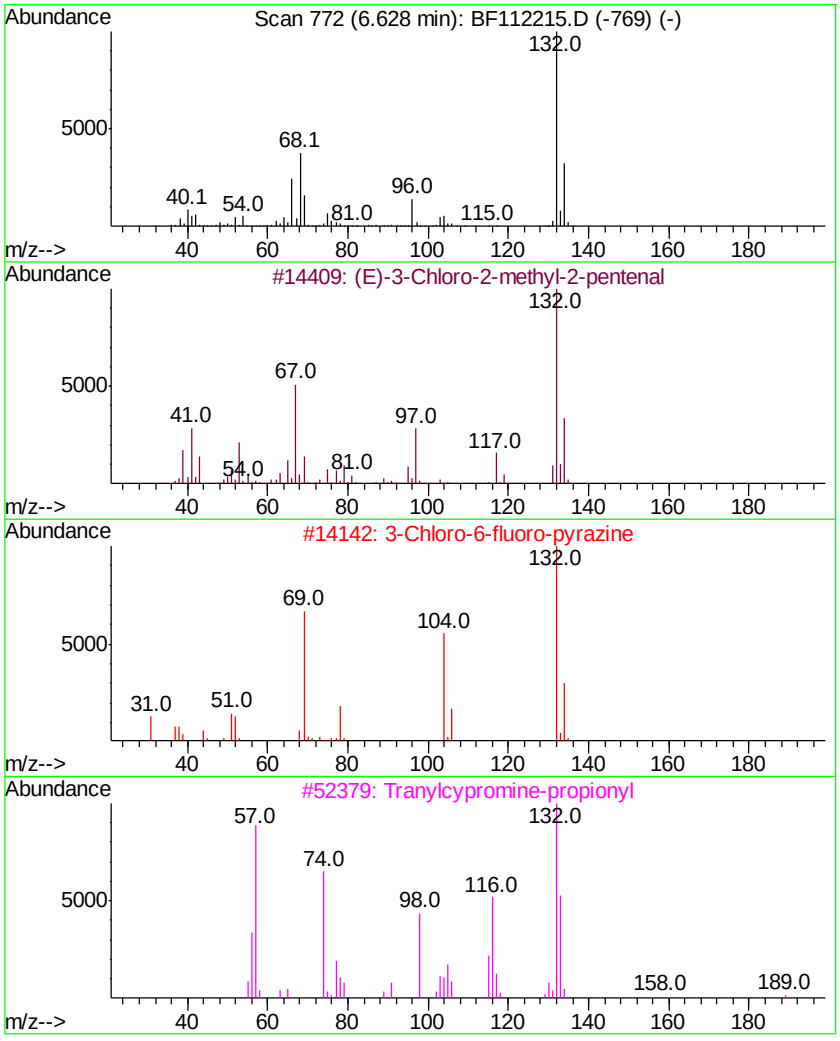
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

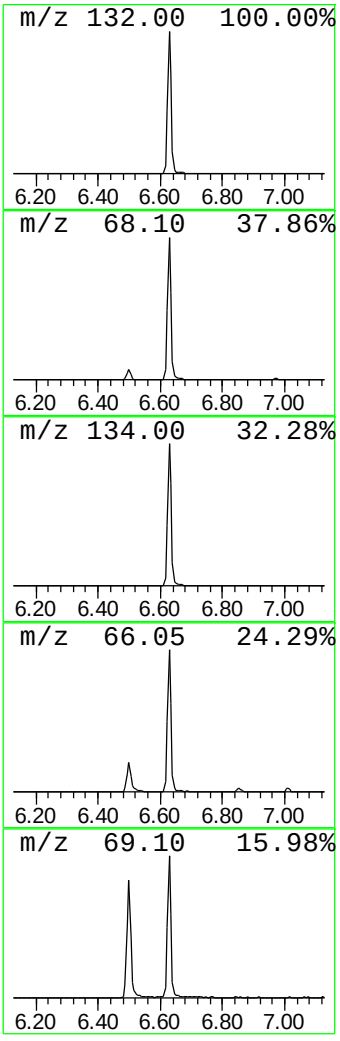
****

Peak Number 1 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	28.89 ng	1985680	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TS-O

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.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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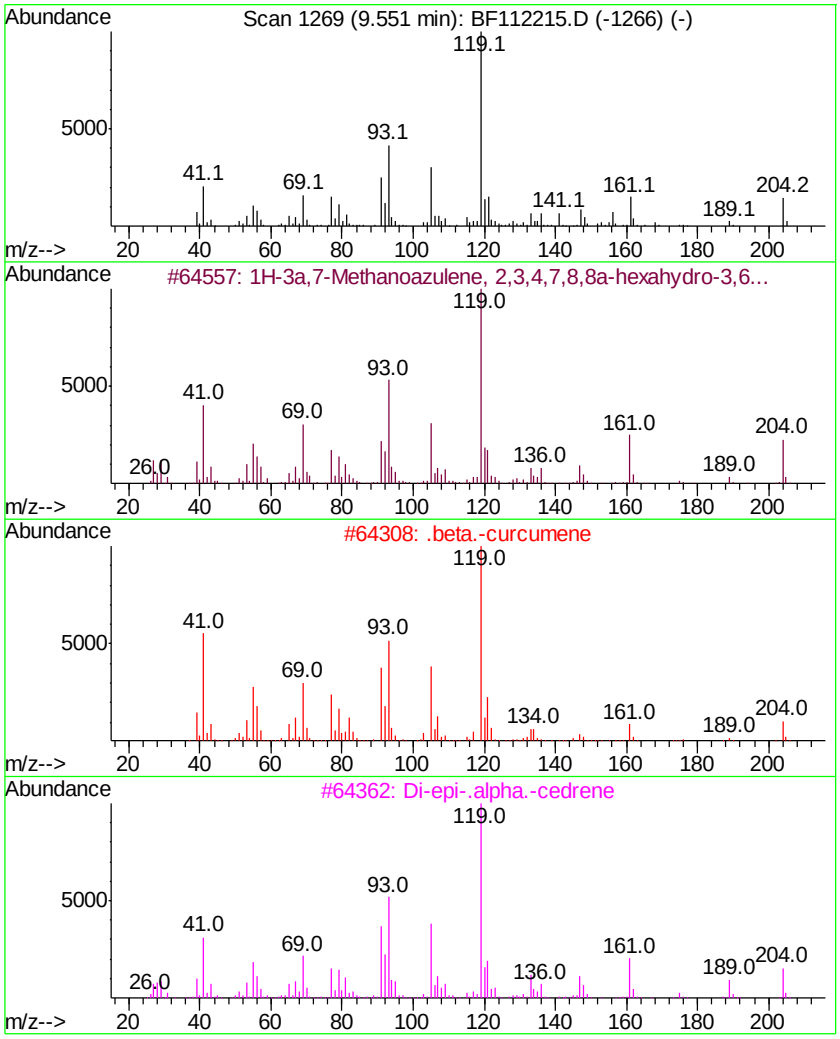
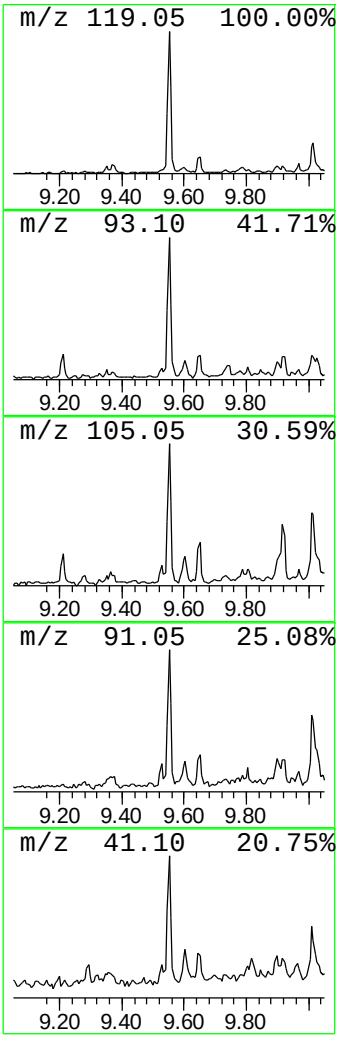
Peak Number 3 1H-3a,7-Methanoazulene, 2,3... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.55	2.96 ng	303203	Acenaphthene-d10	9.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-3a,7-Methanoazulene, 2,3,4,7,...	204	C15H24	000469-61-4	98
2	.beta.-curcumene	204	C15H24	1000374-17-4	87
3	Di-epi-.alpha.-cedrene	204	C15H24	050894-66-1	55
4	Benzene, 1-(1,5-dimethylhexyl)-4...	204	C15H24	001461-02-5	49
5	1,3-Dithiane, 2-(tetrahydrofuran...	204	C8H12O2S2	1000197-25-4	43





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Sample : K1223-03 2X
Misc :
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Instrument : BNA_F
ClientSampleId : TS-O

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.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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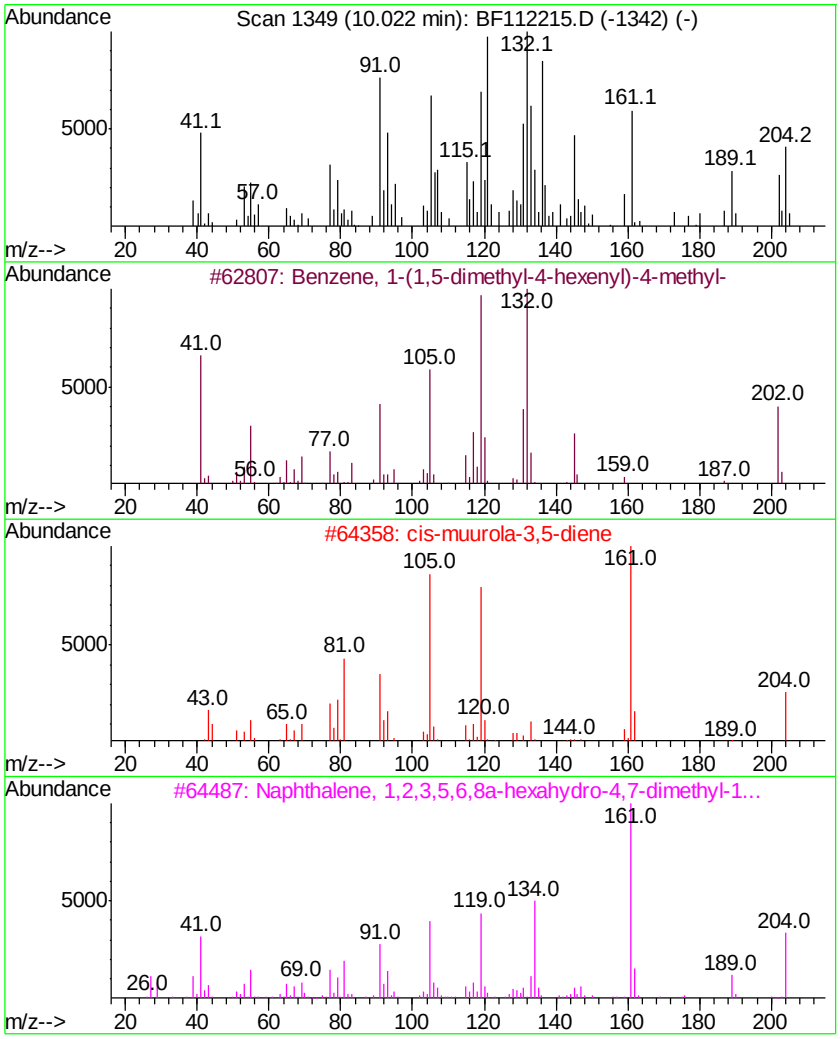
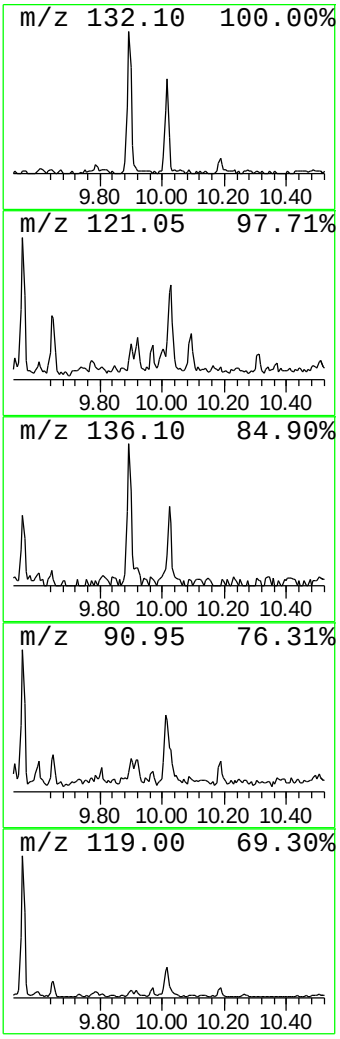
Peak Number 4 Benzene, 1-(1,5-dimethyl-4-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.02	2.67 ng	273843	Acenaphthene-d10	9.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-(1,5-dimethyl-4-hexen...	202	C15H22	000644-30-4	64
2	cis-muurola-3,5-diene	204	C15H24	1000365-95-4	60
3	Naphthalene, 1,2,3,5,6,8a-hexahy...	204	C15H24	000483-76-1	50
4	Benzene, 1-methyl-4-(1,2,2-trime...	202	C15H22	016982-00-6	50
5	.gamma.-Muurolene	204	C15H24	030021-74-0	47





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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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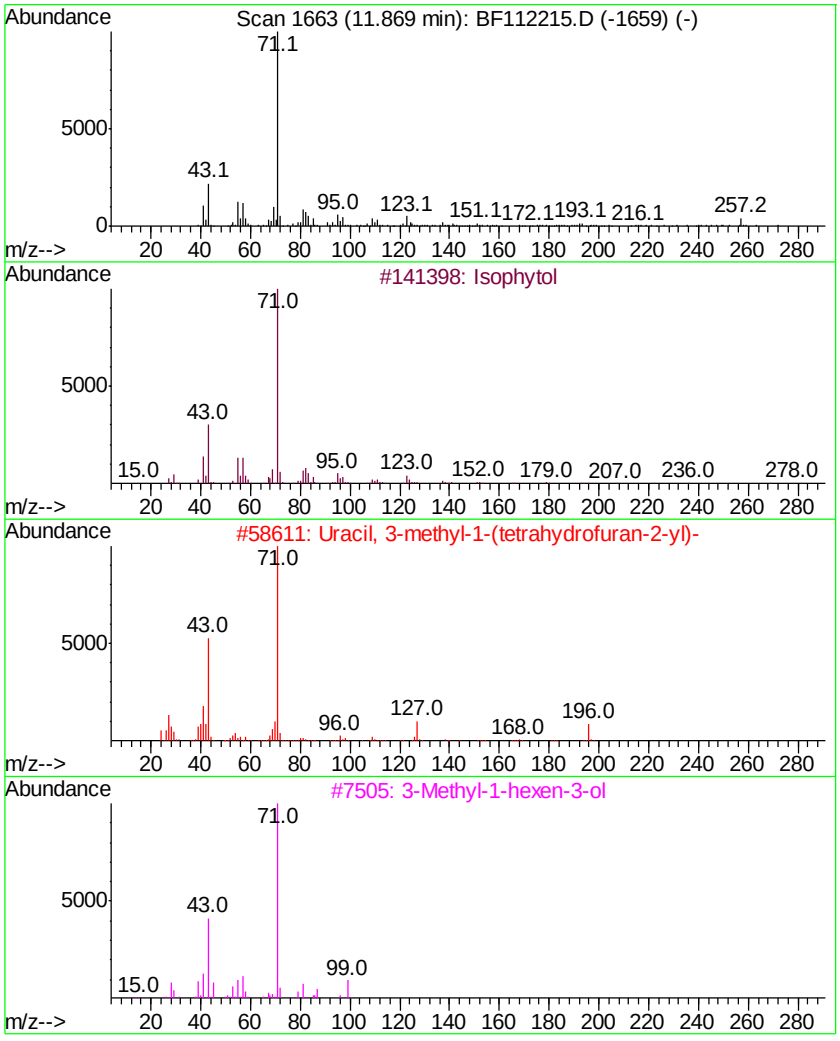
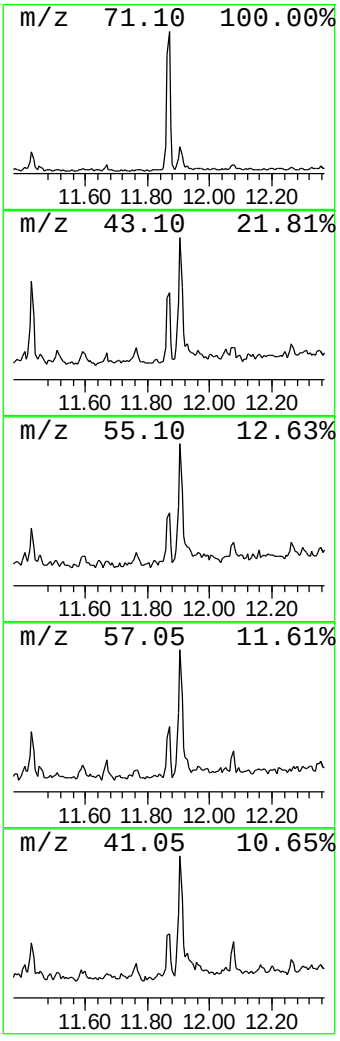
Peak Number 5 Isophytol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	3.87 ng	323940	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isophytol	296	C20H40O	000505-32-8	91
2	Uracil, 3-methyl-1-(tetrahydrofu...	196	C9H12N2O3	1000151-99-4	59
3	3-Methyl-1-hexen-3-ol	114	C7H14O	055145-28-3	53
4	Hexanoic acid, 2-tetrahydrofuryl...	200	C11H20O3	002217-34-7	53
5	6-Bromohexanoic acid, 2-tetrahyd...	278	C11H19BrO3	1000282-30-9	50





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

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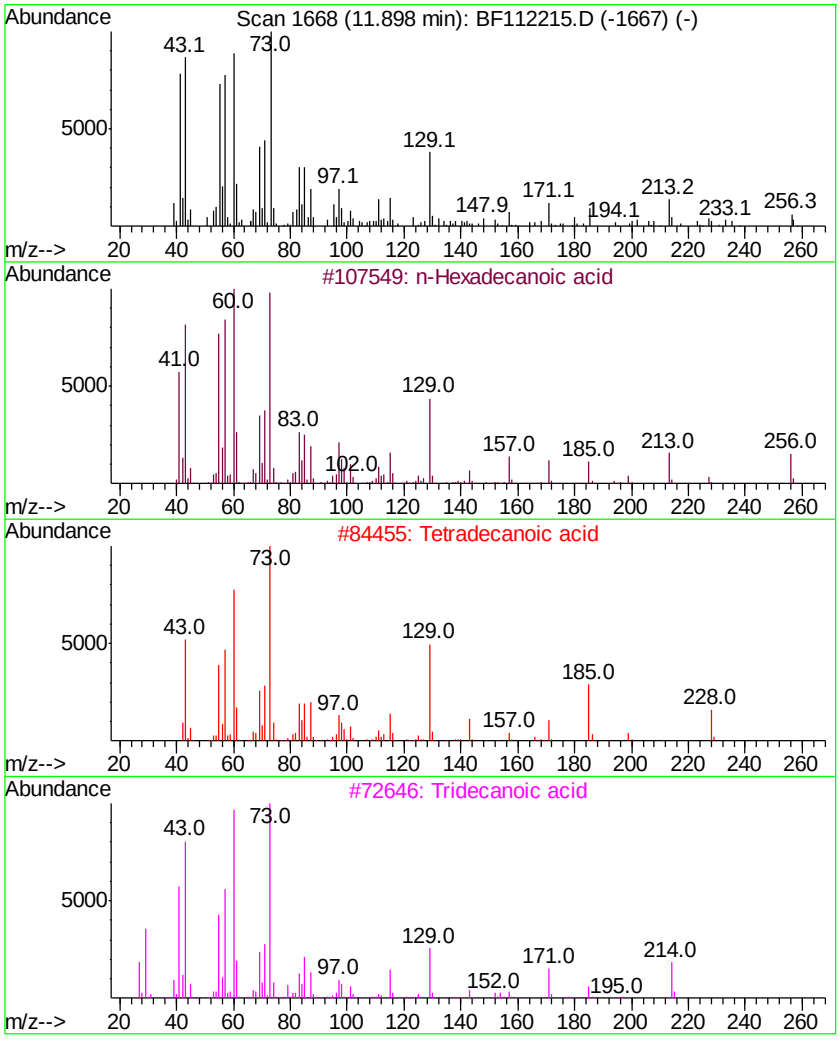
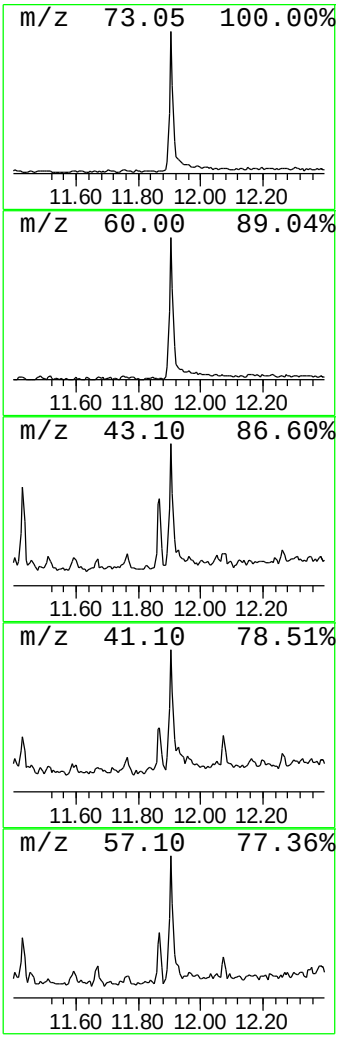
Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	5.83 ng	488279	Phenanthrene-d10	11.38

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	89
3	Tridecanoic acid	214	C13H26O2	000638-53-9	89
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5	Dodecanoic acid	200	C12H24O2	000143-07-7	68





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Sample : K1223-03 2X
Misc :
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Instrument : BNA_F
ClientSampleId : TS-O

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.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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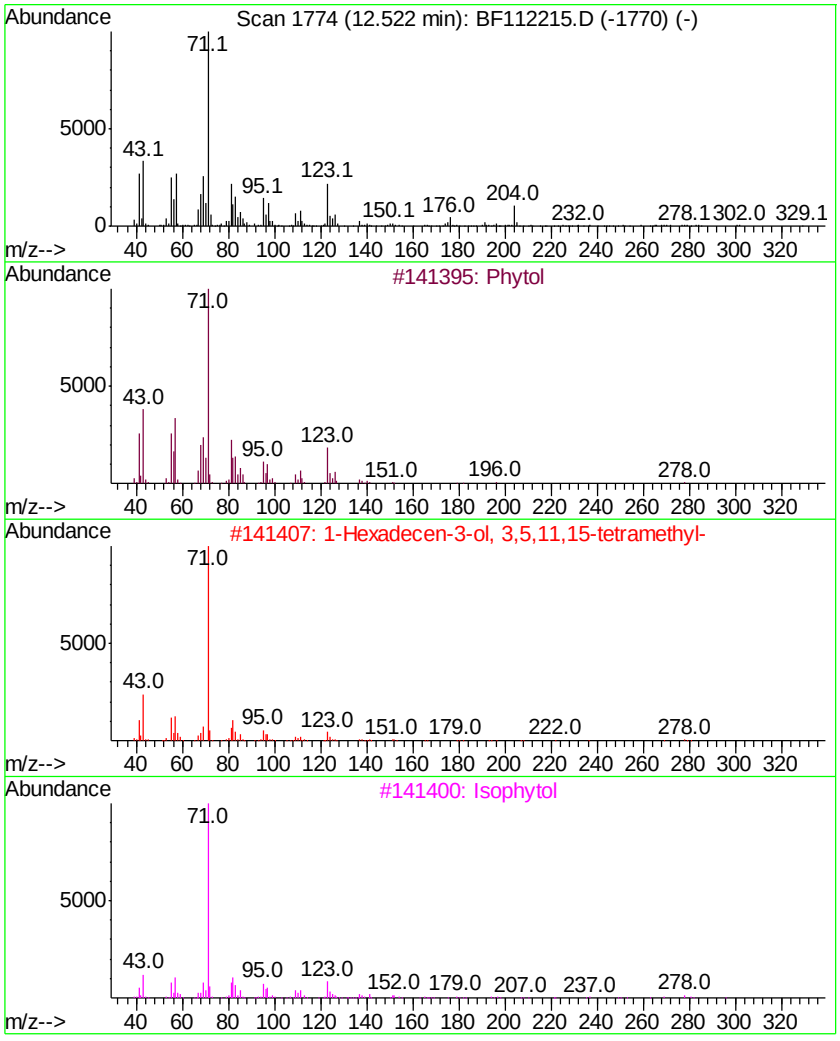
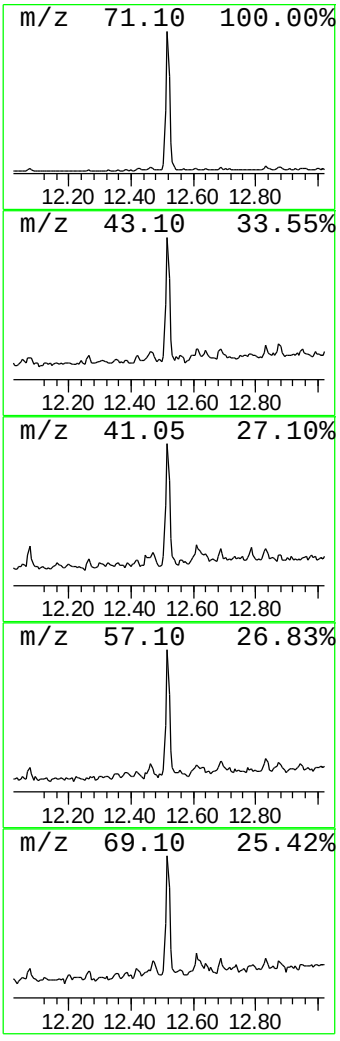
Peak Number 8 Phytol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.52	7.75 ng	648692	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phytol	296	C20H40O	000150-86-7	91
2	1-Hexadecen-3-ol, 3,5,11,15-tetr...	296	C20H40O	1000262-55-5	72
3	Isophytol	296	C20H40O	000505-32-8	72
4	Sulfurous acid, octadecyl 2-pent...	404	C23H48O3S	1000309-16-6	50
5	Butyric acid, 2-pentadecyl ester	298	C19H38O2	107853-73-6	50





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Sample : K1223-03 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TS-O

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

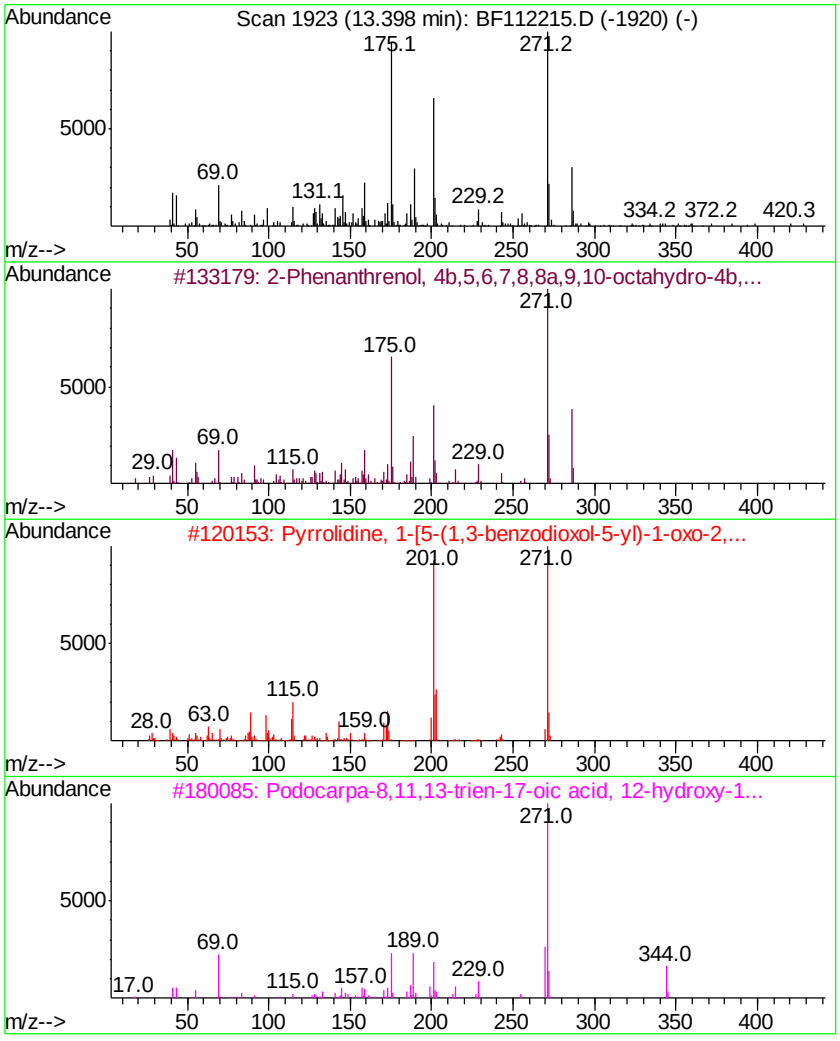
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

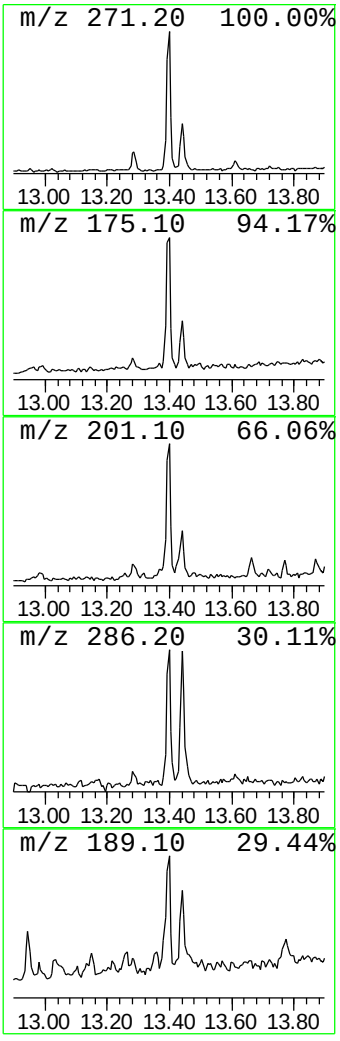
****

Peak Number 9 2-Phenanthrenol, 4b,5,6,7,8... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.40	2.93 ng	230957	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	92
2	Pyrrolidine, 1-[5-(1,3-benzodiox...	271	C16H17NO3	025924-78-1	38
3	Podocarpa-8,11,13-trien-17-oic a...	344	C22H32O3	024067-43-4	38
4	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	328	C22H32O2	015340-82-6	32
5	2,2-Bis(4'-methoxyphenyl)-2-etho...	286	C18H22O3	1000283-53-7	27





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012419\
Data File : BF112215.D
Acq On : 24 Jan 2019 18:10
Operator : JU/SJ
Sample : K1223-03 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TS-O

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

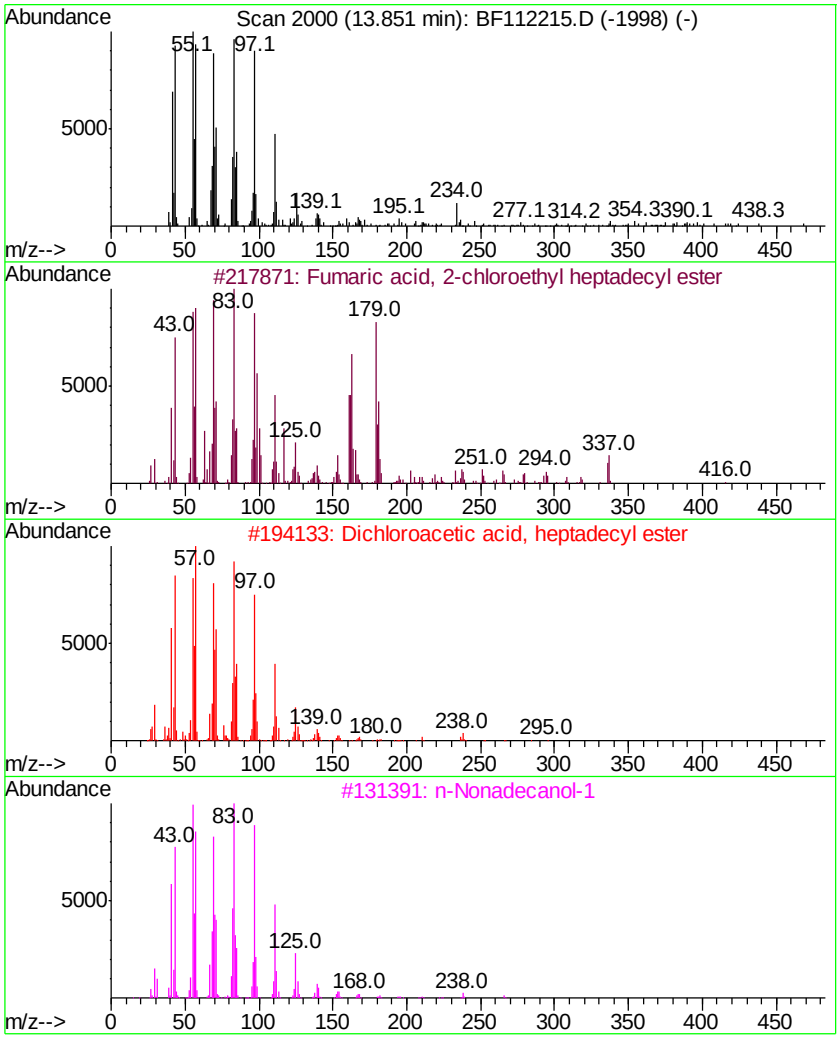
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

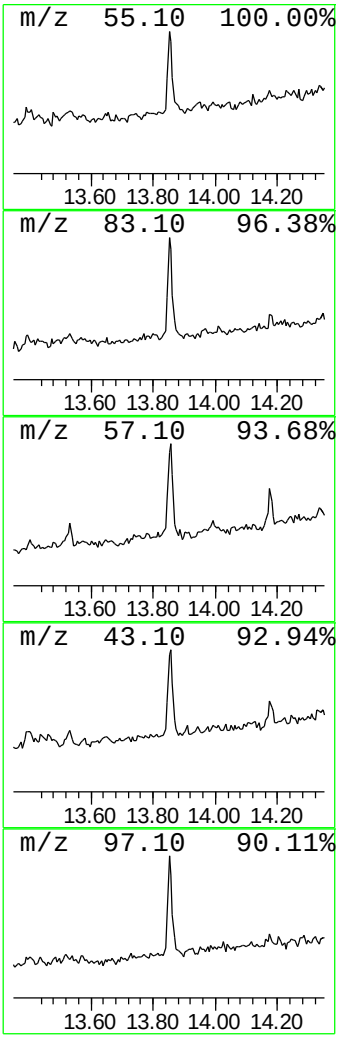
****

Peak Number 10 Fumaric acid, 2-chloroethyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	4.41 ng	347255	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fumaric acid, 2-chloroethyl hept...	416	C23H41ClO4	1000330-62-3	96
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	93
4	Behenic alcohol	326	C22H46O	000661-19-8	93
5	1-Hexadecanol	242	C16H34O	036653-82-4	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012419\
Data File : BF112215.D
Acq On : 24 Jan 2019 18:10
Operator : JU/SJ
Sample : K1223-03 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TS-O

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.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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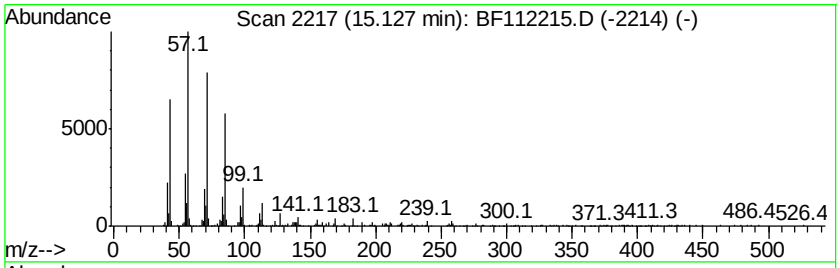
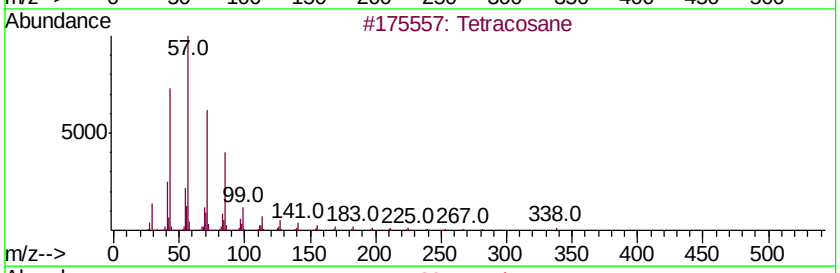
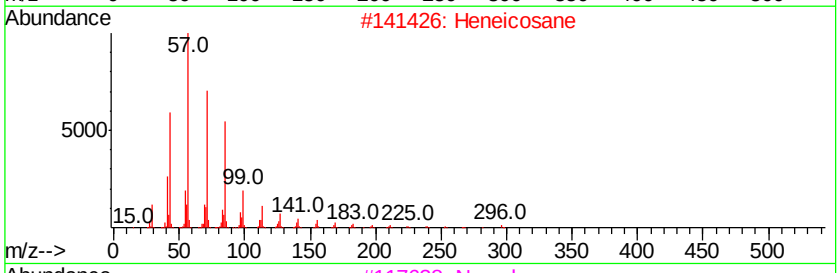
Peak Number 11 Tetracosane Concentration Rank 5

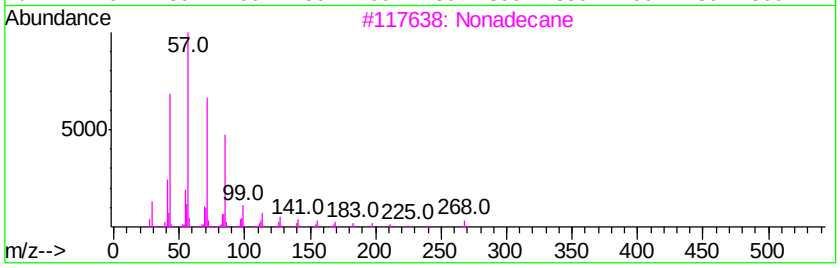
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.13	5.69 ng	323157	Perylene-d12	15.50

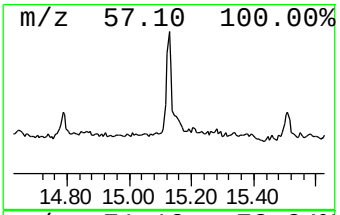
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	94
2	Heneicosane	296	C21H44	000629-94-7	91
3	Nonadecane	268	C19H40	000629-92-5	83
4	Tridecane, 6-propyl-	226	C16H34	055045-10-8	83
5	Hexadecane	226	C16H34	000544-76-3	80

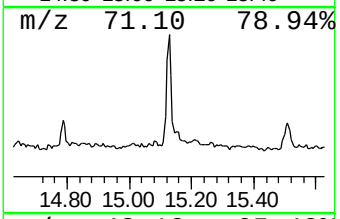


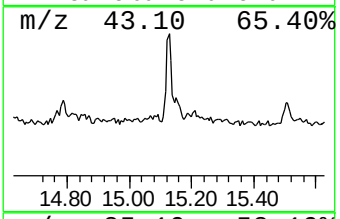


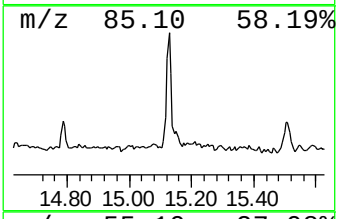


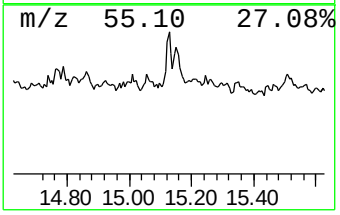












Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF012419\
Data File : BF112215.D
Acq On : 24 Jan 2019 18:10
Operator : JU/SJ
Sample : K1223-03 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.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
unknown6.63	6.63	28.9	ng	1985680	1	6.85	1374500	20.0
1H-3a,7-Methanoaz...	9.55	3.0	ng	303203	3	9.89	2049780	20.0
Benzene, 1-(1,5-d...	10.02	2.7	ng	273843	3	9.89	2049780	20.0
Isophytol	11.87	3.9	ng	323940	4	11.38	1674840	20.0
n-Hexadecanoic acid	11.90	5.8	ng	488279	4	11.38	1674840	20.0
Phytol	12.52	7.8	ng	648692	4	11.38	1674840	20.0
2-Phenanthrenol, ...	13.40	2.9	ng	230957	5	14.03	1575500	20.0
Fumaric acid, 2-c...	13.85	4.4	ng	347255	5	14.03	1575500	20.0
Tetracosane	15.13	5.7	ng	323157	6	15.50	1135980	20.0