LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090222\
Data File : BF130120.D
Acq On : 02 Sep 2022 19:58
Operator : CG\JU
Sample : N4455-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
KTS2-WC-L-MH-02

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-BF083122.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130120.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.628	223	228	232	rBV	49433	73981	1.53%	0.135%
2	3.675	232	236	244	rVB3	44951	68327	1.42%	0.125%
3	4.310	337	344	348	rBV4	38382	105471	2.19%	0.193%
4	4.898	437	444	451	rVB	273430	337622	7.00%	0.618%
5	4.998	451	461	463	rBV	39951	82824	1.72%	0.152%
6	5.081	468	475	497	rVB2	268414	784016	16.26%	1.435%
7	5.304	508	513	516	rBV	2375818	2256262	46.81%	4.130%
8	5.681	575	577	579	rBV	130058	108909	2.26%	0.199%
9	5.716	579	583	589	rVB3	77734	116573	2.42%	0.213%
10	5.869	602	609	612	rBV2	78233	80578	1.67%	0.148%
11	6.328	683	687	692	rVB	1660489	1621013	33.63%	2.967%
12	6.557	722	726	730	rBV2	79247	133343	2.77%	0.244%
13	6.610	730	735	737	rVB3	65366	91451	1.90%	0.167%
14	6.704	747	751	754	rBV	1381150	1225800	25.43%	2.244%
15	6.745	754	758	764	rVB2	86610	100309	2.08%	0.184%
16	6.881	774	781	784	rBV2	79705	109675	2.28%	0.201%
17	7.051	804	810	816	rBV2	61447	107783	2.24%	0.197%
18	7.104	816	819	822	rBV	56410	71276	1.48%	0.130%
19	7.269	839	847	849	rBV	2577393	2637113	54.71%	4.827%
20	7.716	913	923	930	rVB	177876	346319	7.18%	0.634%
21	7.922	953	958	961	rBV3	128025	232104	4.82%	0.425%
22	7.945	961	962	964	rVV	123012	78925	1.64%	0.144%
23	7.981	964	968	972	rVB	1891894	1627137	33.76%	2.979%
24	8.228	1005	1010	1013	rBV2	53258	75388	1.56%	0.138%
25	8.328	1025	1027	1031	rBV4	58807	67090	1.39%	0.123%
26	8.557	1063	1066	1072	rVB2	98697	86184	1.79%	0.158%
27	8.616	1073	1076	1079	rBV2	59252	73236	1.52%	0.134%
28	8.692	1086	1089	1093	rBV2	136287	179118	3.72%	0.328%
29	8.769	1095	1102	1113	rVB2	2919254	2884799	59.85%	5.281%
30	8.892	1120	1123	1128	rVV	347876	315111	6.54%	0.577%
31	8.939	1128	1131	1134	rVB	320654	272223	5.65%	0.498%
32	9.063	1147	1152	1155	rBV	5188483	4820422	100.00%	8.824%
33	9.186	1167	1173	1177	rBV7	155309	253087	5.25%	0.463%
34	9.228	1177	1180	1184	rVB2	115318	132113	2.74%	0.242%
35	9.333	1195	1198	1200	rBV4	48885	66728	1.38%	0.122%
36	9.392	1205	1208	1214	rVV2	440560	598491	12.42%	1.096%

LSC Area Percent Report

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Operator : CG\JU
Sample : N4455-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
KTS2-WC-L-MH-02

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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	9.463	1214	1220	1223	rVV	2589562	2527685	52.44%	4.627%
38	9.492	1223	1225	1229	rVB4	55125	64578	1.34%	0.118%
39	9.563	1232	1237	1240	rVB4	100120	153753	3.19%	0.281%
40	9.604	1240	1244	1245	rBV3	51757	63356	1.31%	0.116%
41	9.657	1251	1253	1255	rVB	116444	72548	1.51%	0.133%
42	9.733	1260	1266	1269	rBV	2297054	1931688	40.07%	3.536%
43	9.763	1269	1271	1275	rVB2	65346	60310	1.25%	0.110%
44	9.804	1275	1278	1281	rBV	143713	125245	2.60%	0.229%
45	9.863	1282	1288	1292	rVB	810850	726053	15.06%	1.329%
46	9.980	1304	1308	1312	rBV2	98796	125823	2.61%	0.230%
47	10.022	1312	1315	1318	rVV	213059	175836	3.65%	0.322%
48	10.145	1333	1336	1340	rBV2	172921	162034	3.36%	0.297%
49	10.192	1340	1344	1347	rVV	642622	591367	12.27%	1.083%
50	10.357	1370	1372	1374	rBV2	69313	72239	1.50%	0.132%
51	10.380	1374	1376	1379	rVB	147264	132528	2.75%	0.243%
52	10.439	1384	1386	1392	rVV2	94551	97645	2.03%	0.179%
53	10.492	1392	1395	1396	rBV	475785	378601	7.85%	0.693%
54	10.522	1396	1400	1411	rVB2	3193671	3966391	82.28%	7.261%
55	10.645	1417	1421	1425	rBV5	158306	278590	5.78%	0.510%
56	10.680	1425	1427	1430	rVB	164897	127225	2.64%	0.233%
57	10.763	1438	1441	1443	rBV	157037	128218	2.66%	0.235%
58	10.822	1445	1451	1453	rBV2	272361	358409	7.44%	0.656%
59	10.945	1466	1472	1474	rBV2	354505	590246	12.24%	1.080%
60	10.969	1474	1476	1483	rVB	1480313	1400202	29.05%	2.563%
61	11.104	1494	1499	1507	rBV4	257611	536046	11.12%	0.981%
62	11.216	1514	1518	1523	rVB	1785812	1666946	34.58%	3.051%
63	11.280	1523	1529	1531	rBV5	112487	183031	3.80%	0.335%
64	11.333	1535	1538	1541	rVB4	66077	66105	1.37%	0.121%
65	11.510	1566	1568	1574	rVB6	62445	97500	2.02%	0.178%
66	11.569	1574	1578	1584	rBV	461234	1072347	22.25%	1.963%
67	11.757	1604	1610	1612	rBV	1533886	1542286	31.99%	2.823%
68	11.774	1612	1613	1617	rVB2	307217	257552	5.34%	0.471%
69	11.845	1622	1625	1628	rVB	103126	109176	2.26%	0.200%
70	11.992	1646	1650	1661	rBV2	326704	682752	14.16%	1.250%
71	12.263	1694	1696	1700	rBV2	129894	109818	2.28%	0.201%
72	12.357	1709	1712	1714	rBV3	53865	57710	1.20%	0.106%
73	12.386	1714	1717	1719	rVB2	106346	94818	1.97%	0.174%
74	12.480	1731	1733	1736	rVB	234431	205020	4.25%	0.375%
75	12.539	1739	1743	1748	rVV	692344	728205	15.11%	1.333%
76	12.798	1783	1787	1790	rBV	3908723	3385509	70.23%	6.197%

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KTS2-WC-L-MH-02

Integration Parameters: rteint.p
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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

77	13.098	1836	1838	1846	rVB6	61536	91075	1.89%	0.167%
78	13.210	1854	1857	1859	rBV2	90619	91492	1.90%	0.167%
79	13.233	1859	1861	1865	rVV3	79114	108967	2.26%	0.199%
80	13.269	1865	1867	1873	rVB3	131590	175577	3.64%	0.321%
81	13.710	1939	1942	1946	rVB	76977	70051	1.45%	0.128%
82	13.763	1947	1951	1959	rBV	605473	1087636	22.56%	1.991%
83	13.839	1961	1964	1968	rVB	1141933	1033728	21.44%	1.892%
84	13.951	1979	1983	1987	rVB2	215213	291866	6.05%	0.534%
85	14.021	1992	1995	2002	rVV2	93614	140355	2.91%	0.257%
86	14.327	2044	2047	2053	rVB	119130	117121	2.43%	0.214%
87	14.410	2058	2061	2070	rVB4	106189	169293	3.51%	0.310%
88	14.621	2094	2097	2102	rVB	115522	112102	2.33%	0.205%
89	14.692	2106	2109	2114	rVB	72458	70738	1.47%	0.129%
90	14.939	2147	2151	2160	rVB	167515	218815	4.54%	0.401%
91	15.245	2198	2203	2207	rBV	896605	1056994	21.93%	1.935%
92	15.286	2207	2210	2219	rVB2	101474	150385	3.12%	0.275%
93	15.692	2275	2279	2287	rVB	108530	168967	3.51%	0.309%
94	15.833	2298	2303	2307	rBV5	66660	152466	3.16%	0.279%
95	16.162	2354	2359	2362	rBV	97450	185955	3.86%	0.340%
96	16.768	2456	2462	2476	rBV9	72078	274067	5.69%	0.502%
97	16.898	2479	2484	2488	rBV7	58513	115565	2.40%	0.212%
98	17.021	2497	2505	2519	rVB7	125583	461626	9.58%	0.845%
99	17.180	2526	2532	2535	rBV5	97617	213169	4.42%	0.390%
100	17.333	2551	2558	2580	rVB6	185761	743359	15.42%	1.361%

Sum of corrected areas: 54627561

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Data File : BF130120.D
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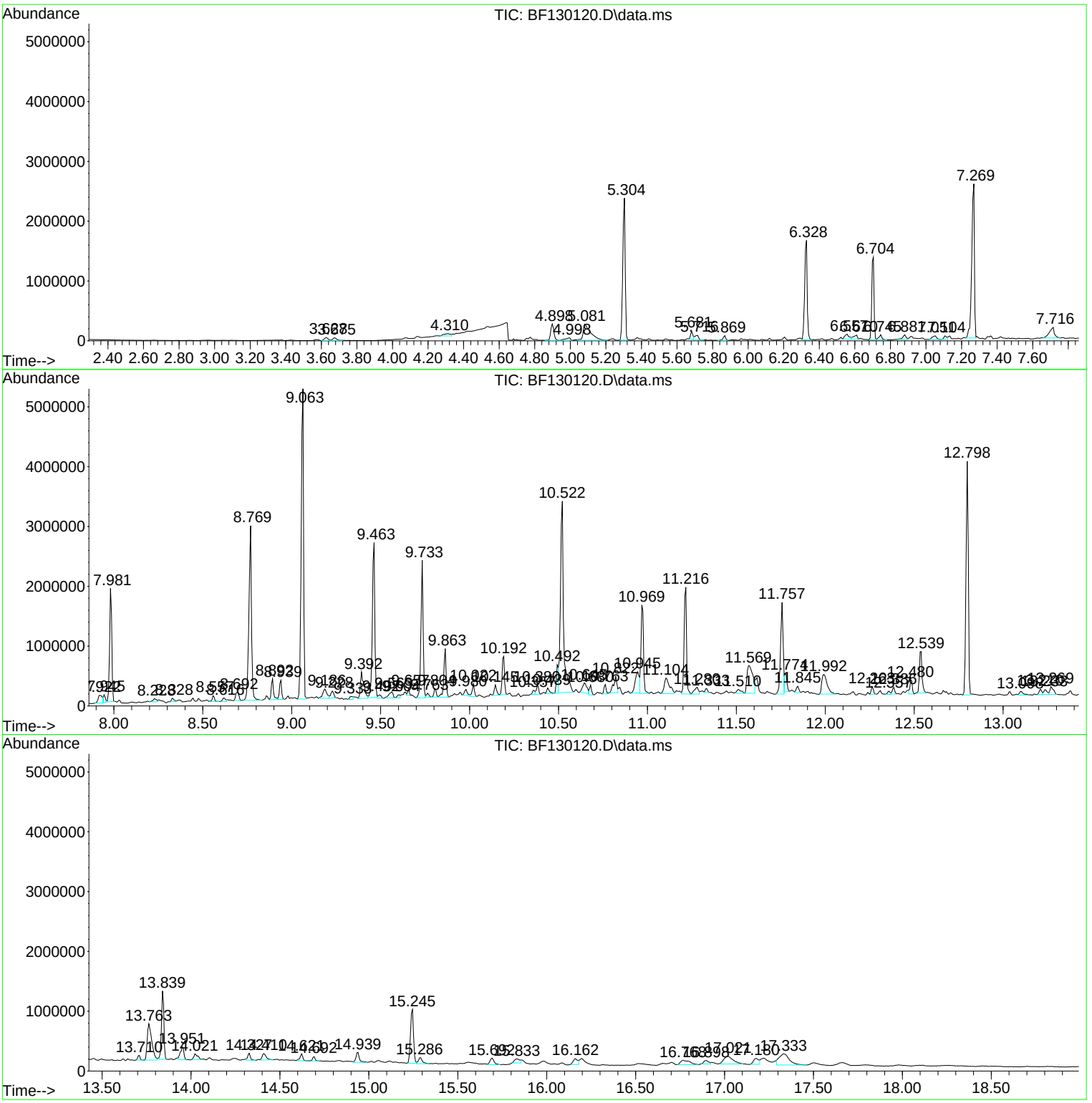
Instrument :
BNA_F
ClientSampleId :
KTS2-WC-L-MH-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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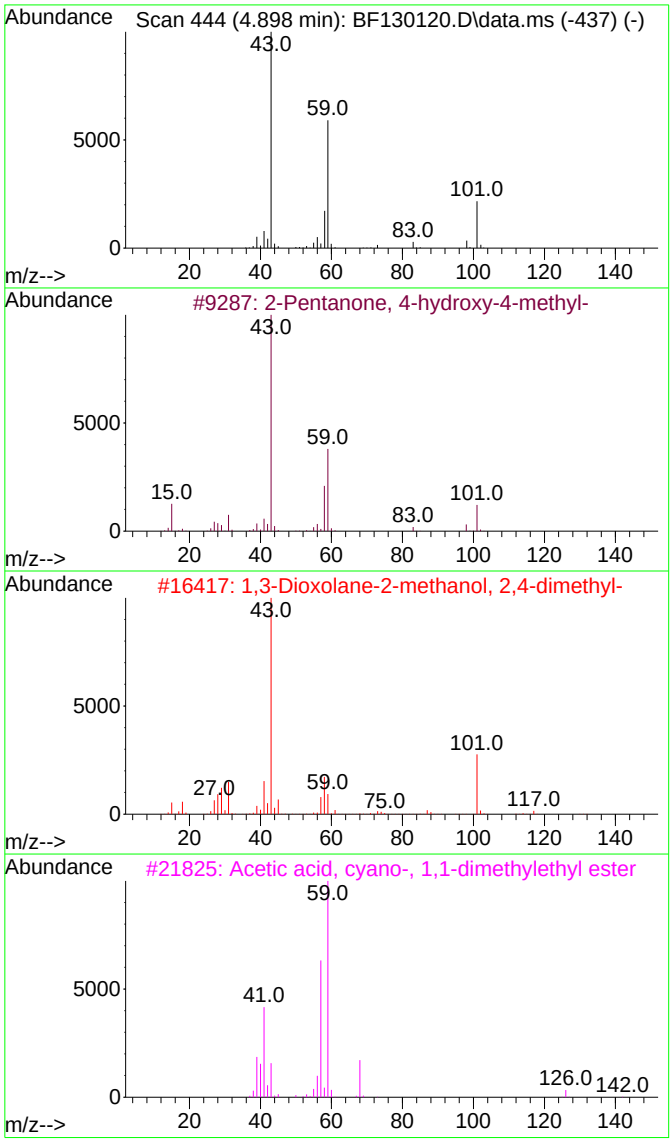
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

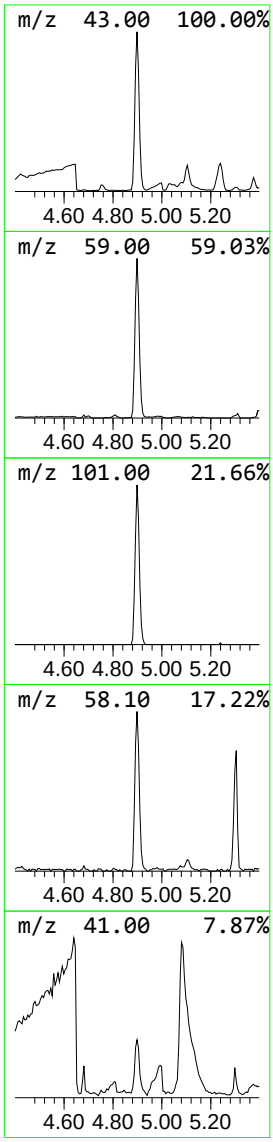
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.898	5.51 ng	337622	1,4-Dichlorobenzene-d4	6.704

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





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KTS2-WC-L-MH-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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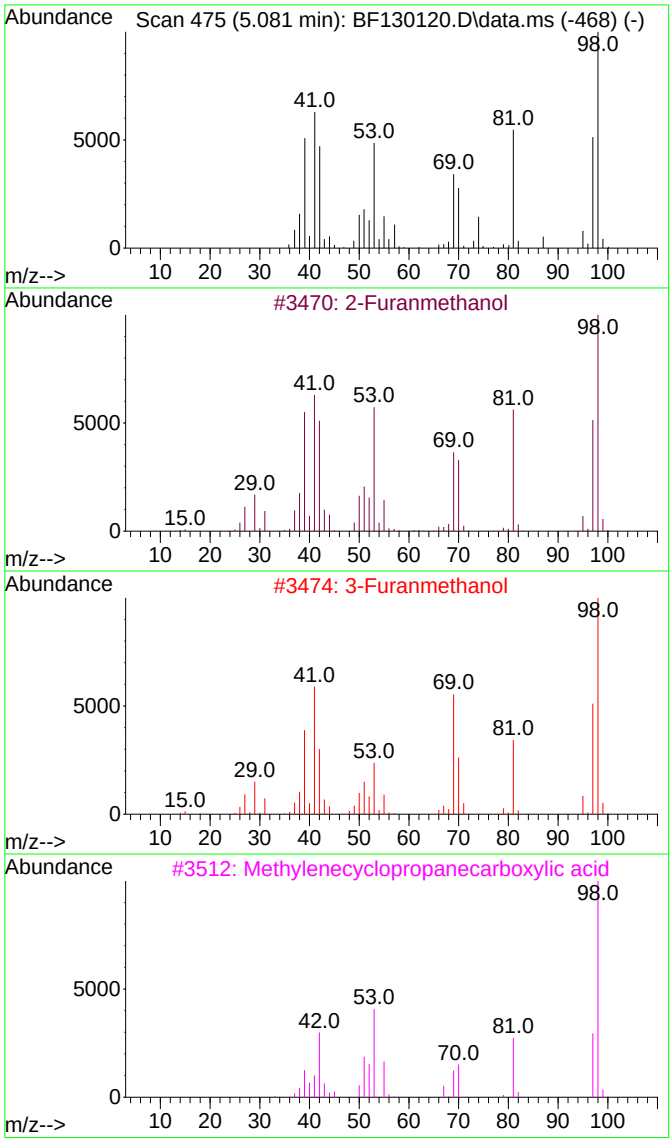
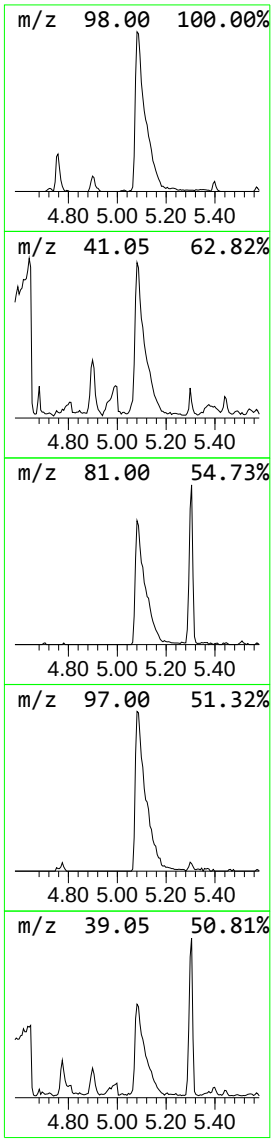
****

Peak Number 2 2-Furanmethanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.081	12.79 ng	784016	1,4-Dichlorobenzene-d4	6.704

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Furanmethanol	98	C5H6O2	000098-00-0	98
2	3-Furanmethanol	98	C5H6O2	004412-91-3	87
3	Methylenecyclopropanecarboxylic ...	98	C5H6O2	062266-36-8	59
4	2,4-Hexadienal, (E,E)-	96	C6H8O	000142-83-6	38
5	N-Methyl-7-azabicyclo(2,2,1)hept...	109	C7H11N	055590-26-6	38





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TIC Library : C:\Database\NIST20.L
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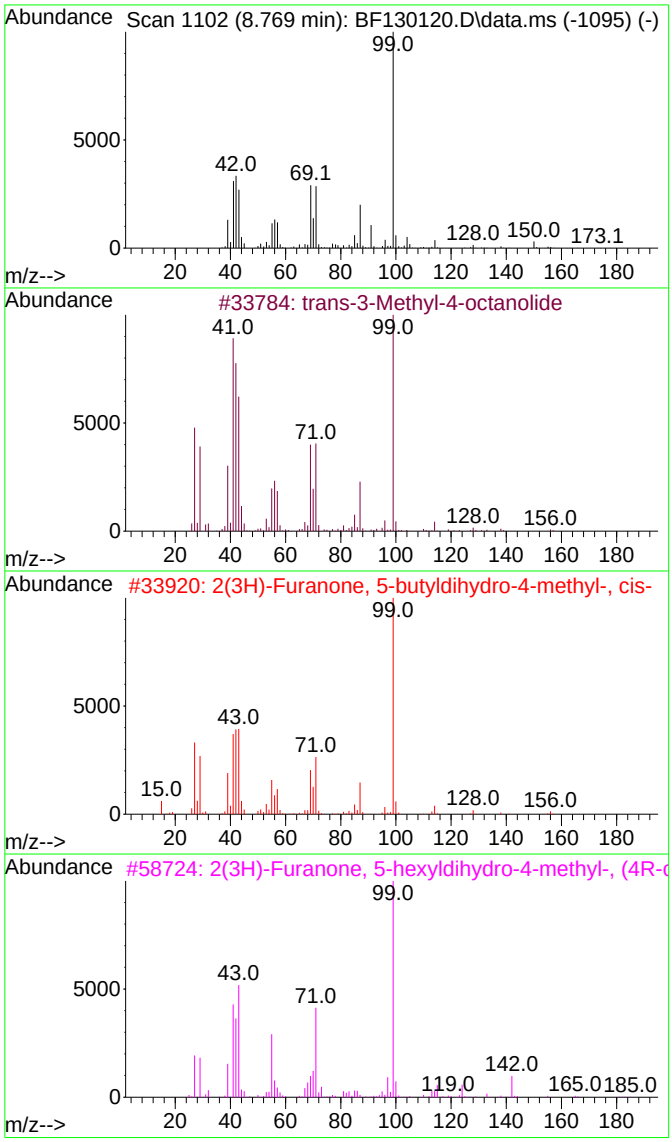
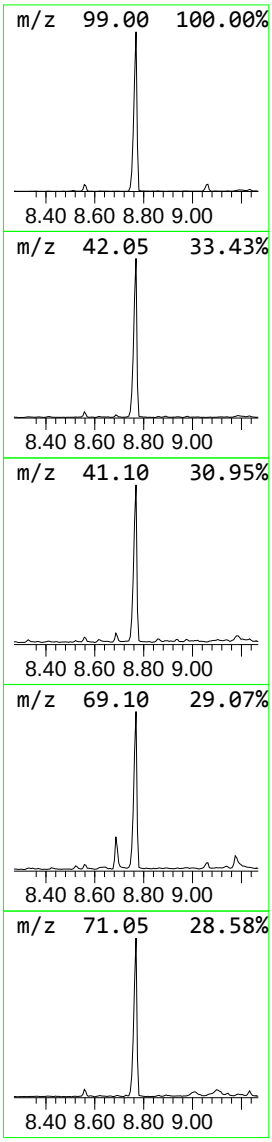
****
Peak Number 3 trans-3-Methyl-4-octanolide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.769	35.46 ng	2884800	Naphthalene-d8	7.981

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-3-Methyl-4-octanolide	156	C9H16O2	039638-67-0	90
2	2(3H)-Furanone, 5-butyldihydro-4...	156	C9H16O2	055013-32-6	72
3	2(3H)-Furanone, 5-hexyldihydro-4...	184	C11H20O2	121644-12-0	59
4	trans-4-Hydroxy-3-methylundecano...	198	C12H22O2	148806-10-4	59
5	cis-4-Hydroxy-3-methylundecanoic...	198	C12H22O2	148806-09-1	53





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TIC Library : C:\Database\NIST20.L
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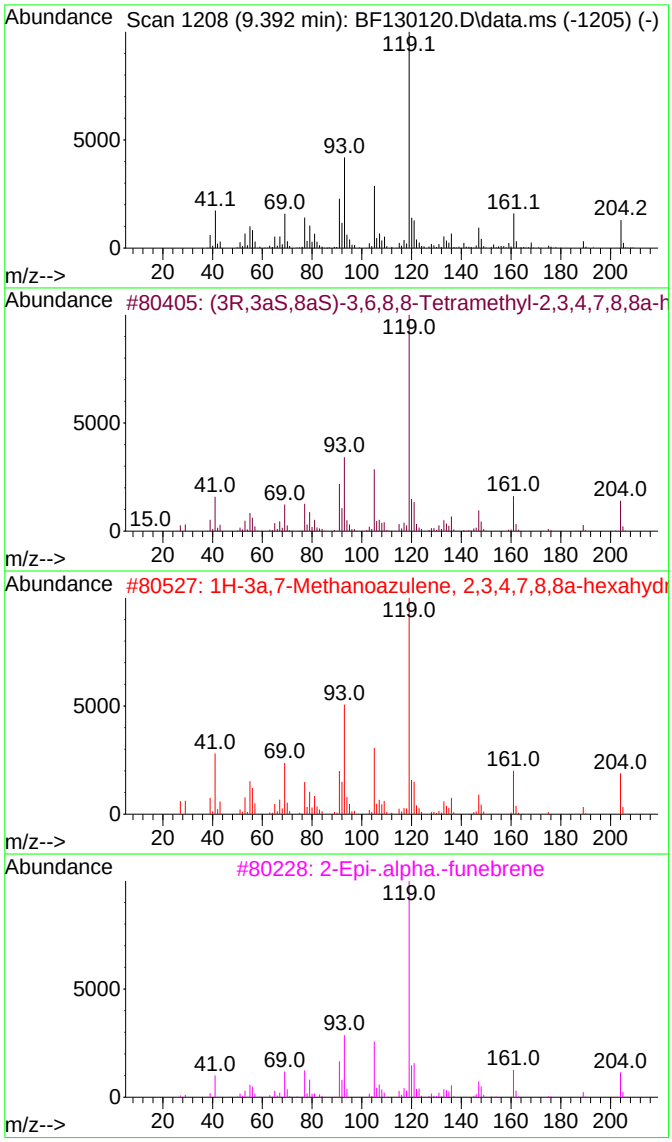
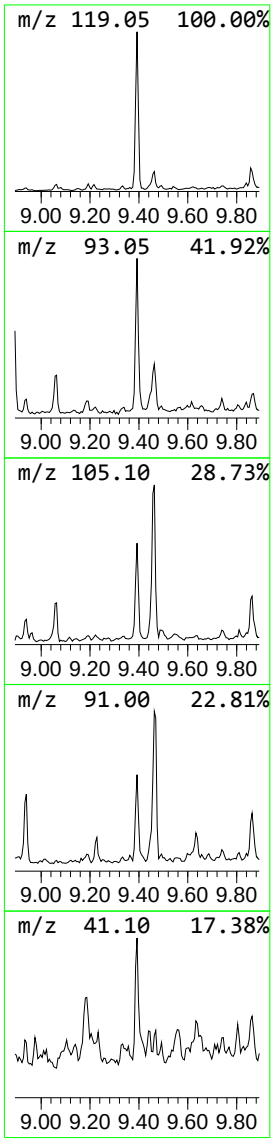
****
Peak Number 4 (3R,3aS,8aS)-3,6,8,8-Tetram... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.392	6.20 ng	598491	Acenaphthene-d10	9.733

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(3R,3aS,8aS)-3,6,8,8-Tetramethyl...	204	C15H24	022567-43-7	99
2	1H-3a,7-Methanoazulene, 2,3,4,7,...	204	C15H24	000469-61-4	99
3	2-Epi-.alpha.-funebrene	204	C15H24	065354-33-8	87
4	(1S,5S)-2-Methyl-5-((R)-6-methyl...	204	C15H24	159407-35-9	87
5	(R)-1-Methyl-4-(6-methylhept-5-e...	204	C15H24	028976-67-2	78





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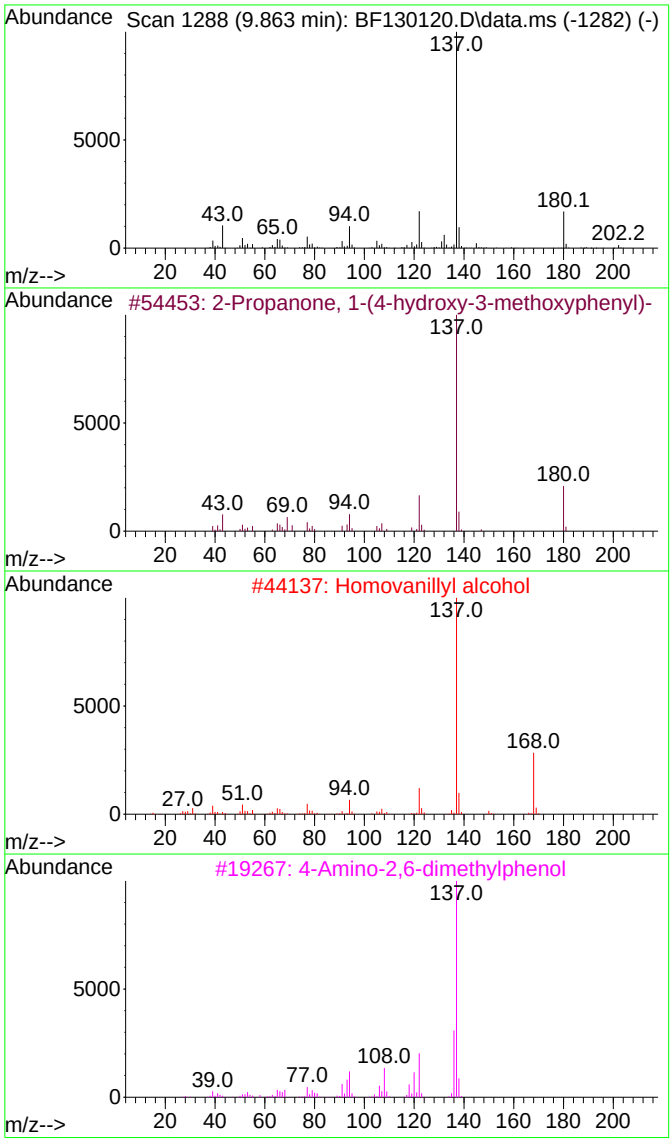
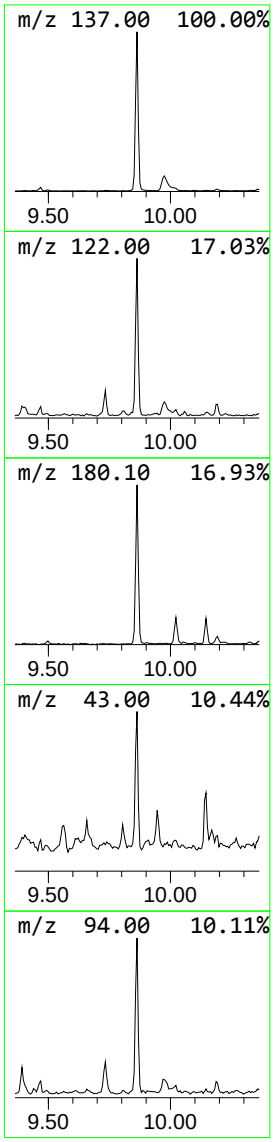
****
Peak Number 5 2-Propanone, 1-(4-hydroxy-3... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.863	7.52 ng	726053	Acenaphthene-d10	9.733

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanone, 1-(4-hydroxy-3-meth...	180	C10H12O3	002503-46-0	90
2	Homovanillyl alcohol	168	C9H12O3	002380-78-1	72
3	4-Amino-2,6-dimethylphenol	137	C8H11NO	015980-22-0	72
4	Homovanillic acid	182	C9H10O4	000306-08-1	64
5	Benzeneacetic acid, 4-hydroxy-3-...	196	C10H12O4	015964-80-4	64





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Sample : N4455-01
Misc :
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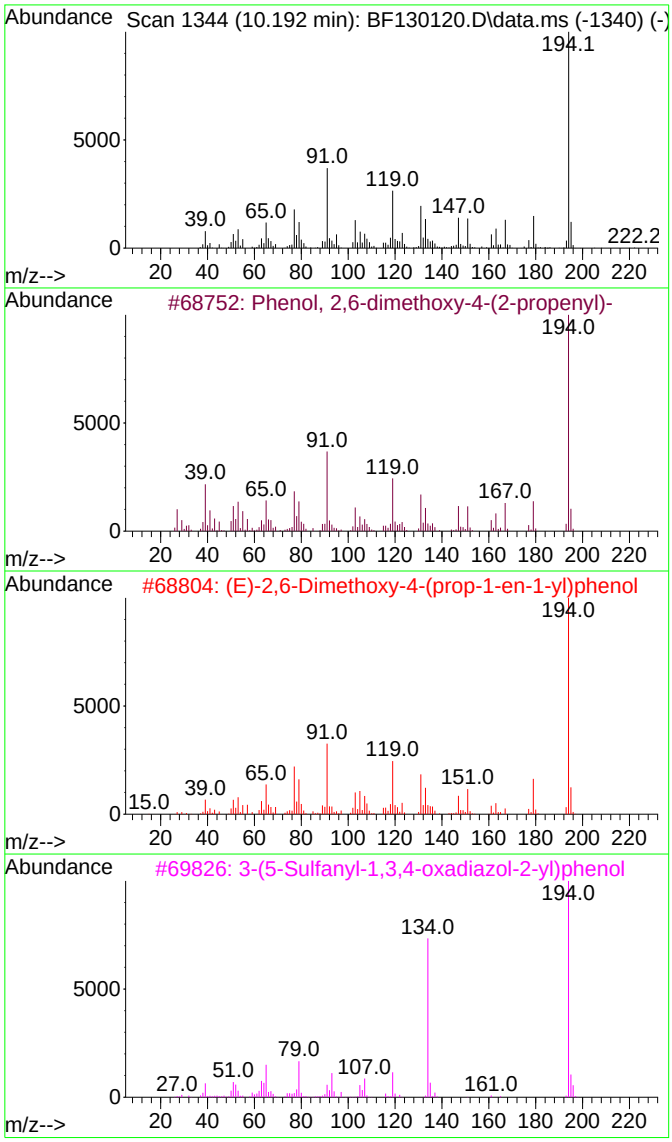
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

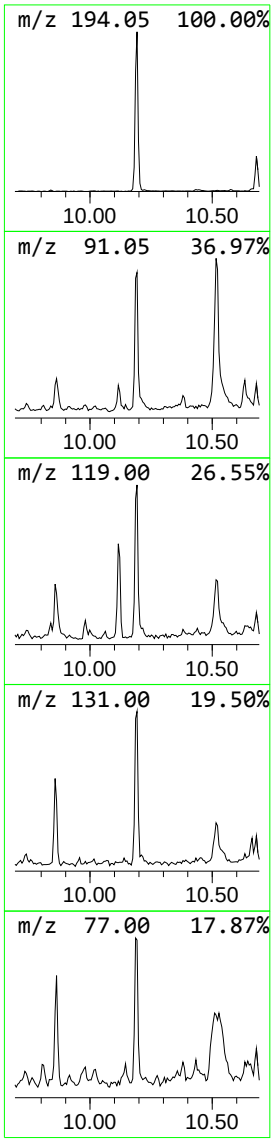
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Phenol, 2,6-dimethoxy-4-(2-... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.192	6.12 ng	591367	Acenaphthene-d10	9.733

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,6-dimethoxy-4-(2-prope...	194	C11H14O3	006627-88-9	99
2	(E)-2,6-Dimethoxy-4-(prop-1-en-1...	194	C11H14O3	020675-95-0	98
3	3-(5-Sulfanyl-1,3,4-oxadiazol-2-...	194	C8H6N2O2S	299465-12-6	43
4	3-Methoxy-4,5-ethylenedioxybenza...	194	C10H10O4	075889-54-2	43
5	Dibenz[c,e]oxepin	194	C14H10O	000219-98-7	43





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ClientSampleId :
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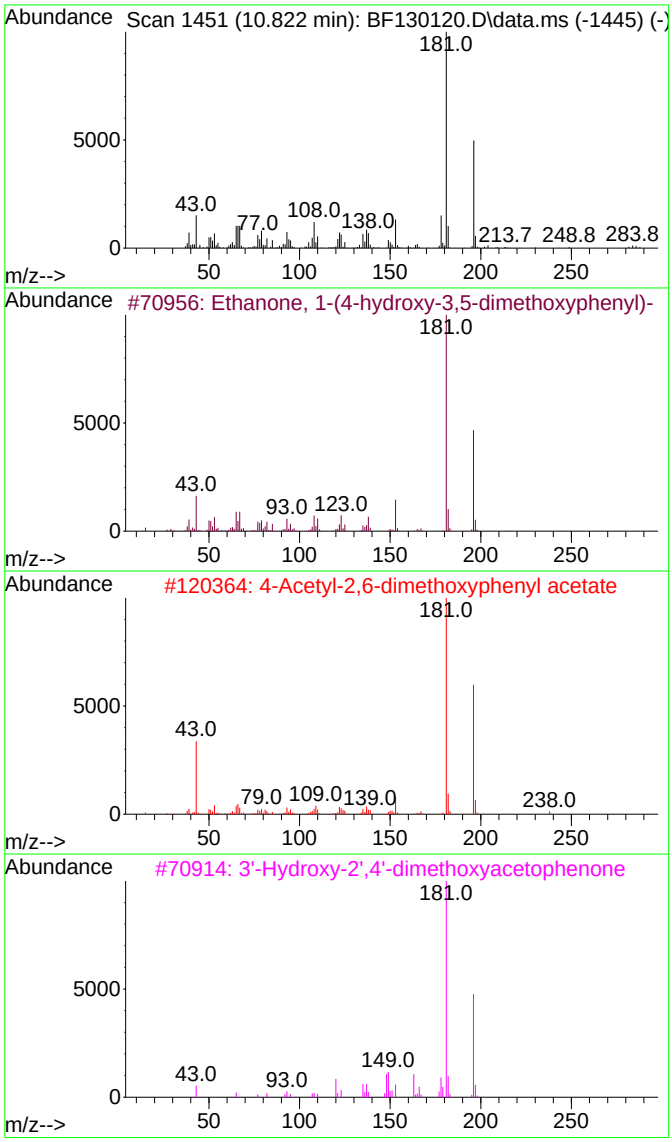
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

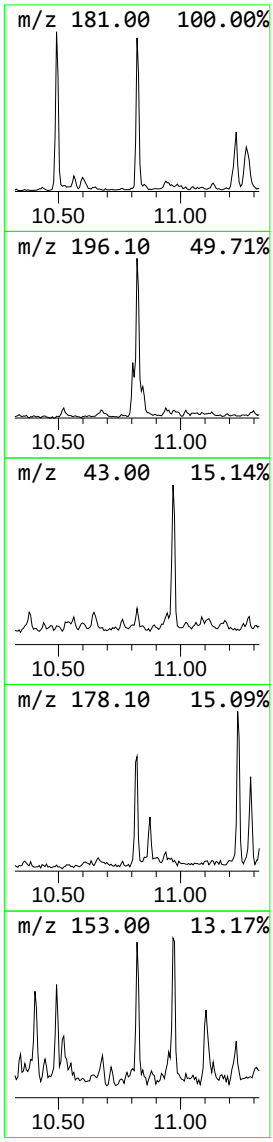
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Ethanone, 1-(4-hydroxy-3,5-... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.822	4.30 ng	358409	Phenanthrene-d10	11.216

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanone, 1-(4-hydroxy-3,5-dimet...	196	C10H12O4	002478-38-8	94
2	4-Acetyl-2,6-dimethoxyphenyl ace...	238	C12H14O5	1000385-76-7	72
3	3'-Hydroxy-2',4'-dimethoxyacetop...	196	C10H12O4	1000433-07-3	72
4	Xanthoxylin	196	C10H12O4	000090-24-4	64
5	2'-Hydroxy-3',4'-dimethoxyacetop...	196	C10H12O4	1000433-07-2	64





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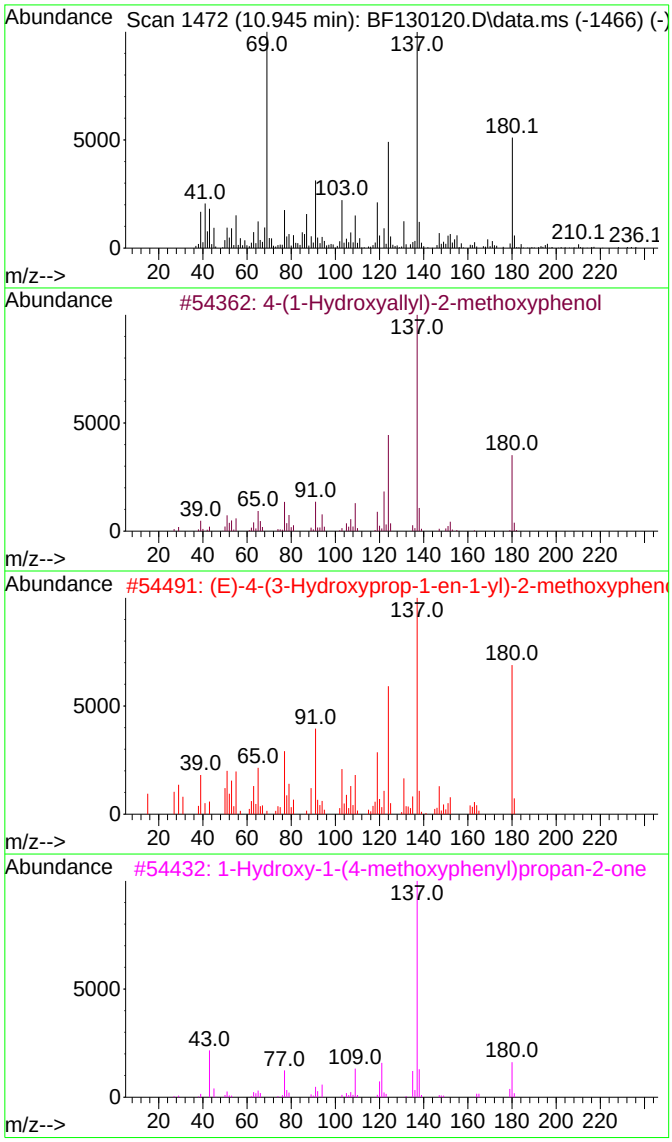
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

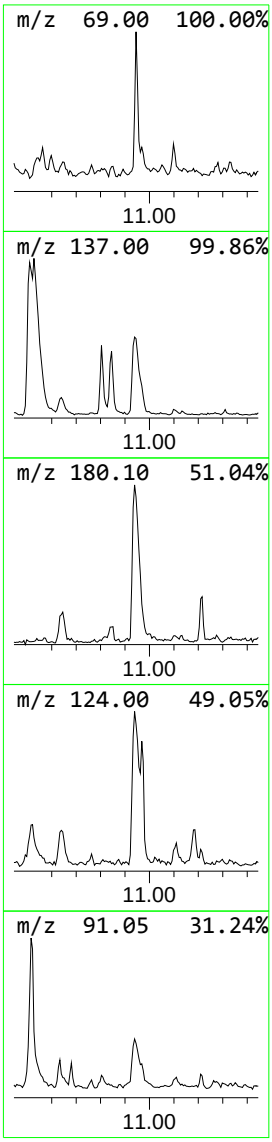
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 4-(1-Hydroxyallyl)-2-methox... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.945	7.08 ng	590246	Phenanthrene-d10	11.216

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-(1-Hydroxyallyl)-2-methoxyphenol	180	C10H12O3	112465-50-6	70
2	(E)-4-(3-Hydroxyprop-1-en-1-yl)-...	180	C10H12O3	032811-40-8	68
3	1-Hydroxy-1-(4-methoxyphenyl)pro...	180	C10H12O3	015482-29-8	41
4	4,8-Dimethylbicyclo[3.3.1]nonane...	180	C11H16O2	139914-54-8	38
5	Pyrazine, 2-methoxy-3-(1-methyle...	152	C8H12N2O	025773-40-4	38





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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

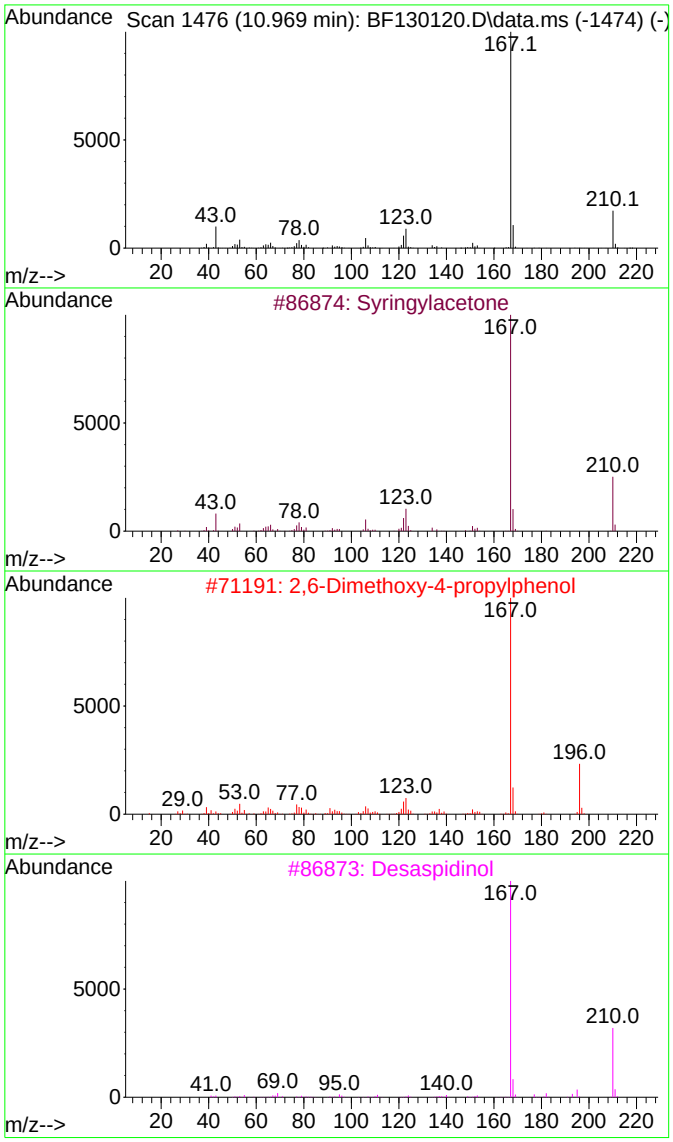
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

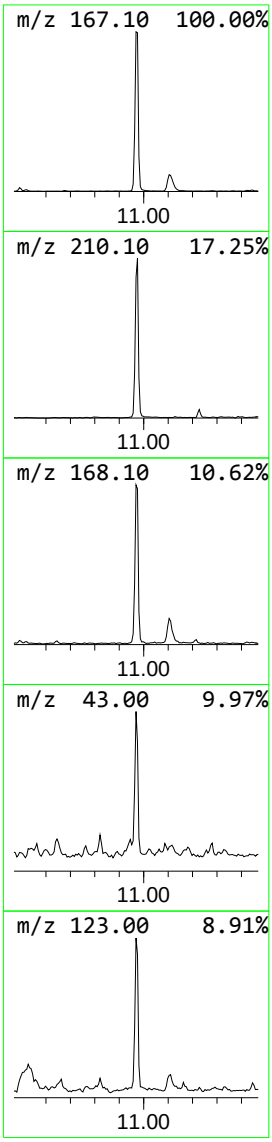
****

Peak Number 9 Syringylacetone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.969	16.80 ng	1400200	Phenanthrene-d10	11.216

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Syringylacetone	210	C11H14O4	019037-58-2	93
2	2,6-Dimethoxy-4-propylphenol	196	C11H16O3	006766-82-1	72
3	Desaspidinol	210	C11H14O4	000437-72-9	72
4	Homosyringaldehyde	196	C10H12O4	087345-52-6	50
5	2-Mercaptobenzothiazole	167	C7H5NS2	000149-30-4	39





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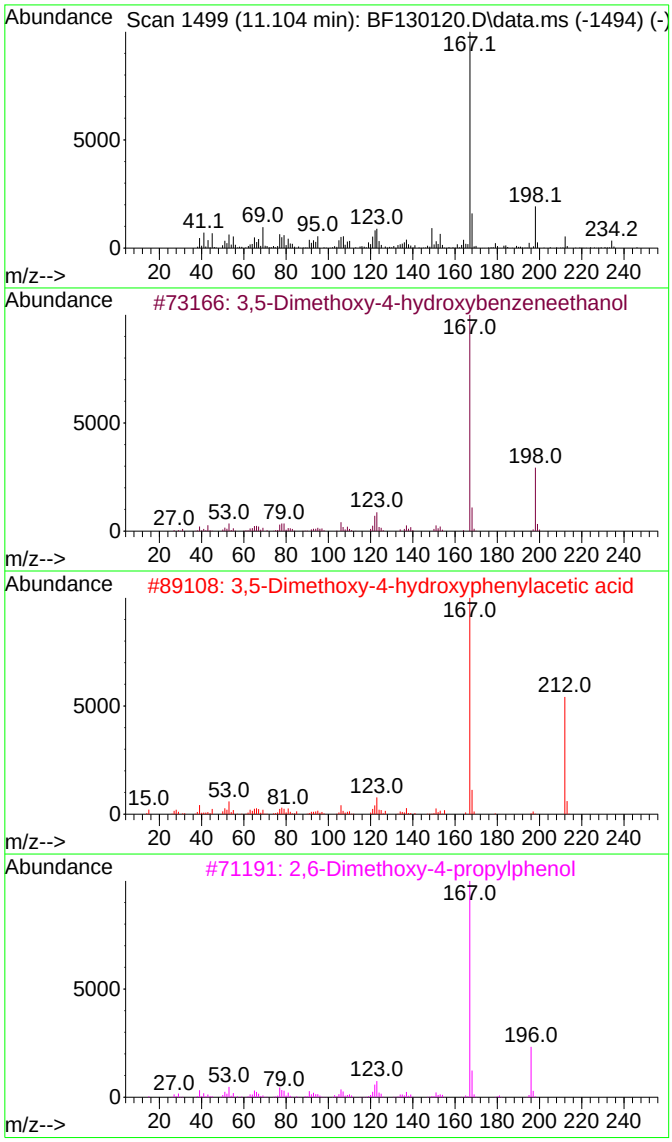
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

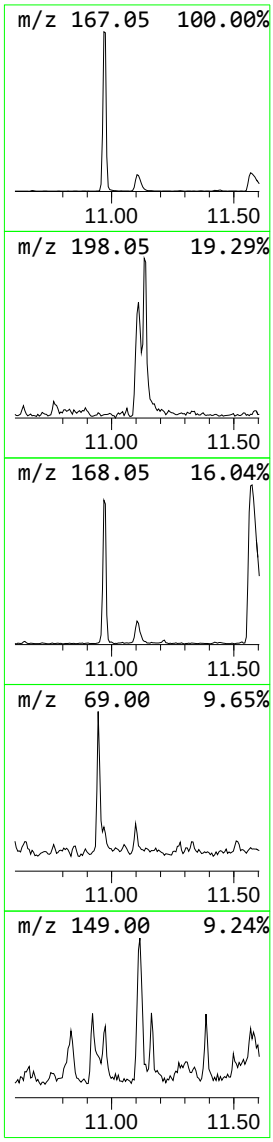
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 3,5-Dimethoxy-4-hydroxybenz... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.104	6.43 ng	536046	Phenanthrene-d10	11.216

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-Dimethoxy-4-hydroxybenzeneet...	198	C10H14O4	020824-45-7	81
2	3,5-Dimethoxy-4-hydroxyphenylace...	212	C10H12O5	004385-56-2	58
3	2,6-Dimethoxy-4-propylphenol	196	C11H16O3	006766-82-1	52
4	Carbazole	167	C12H9N	000086-74-8	52
5	Phenol, 2,4-dimethyl-6-nitro-, a...	209	C10H11NO4	013287-32-6	50





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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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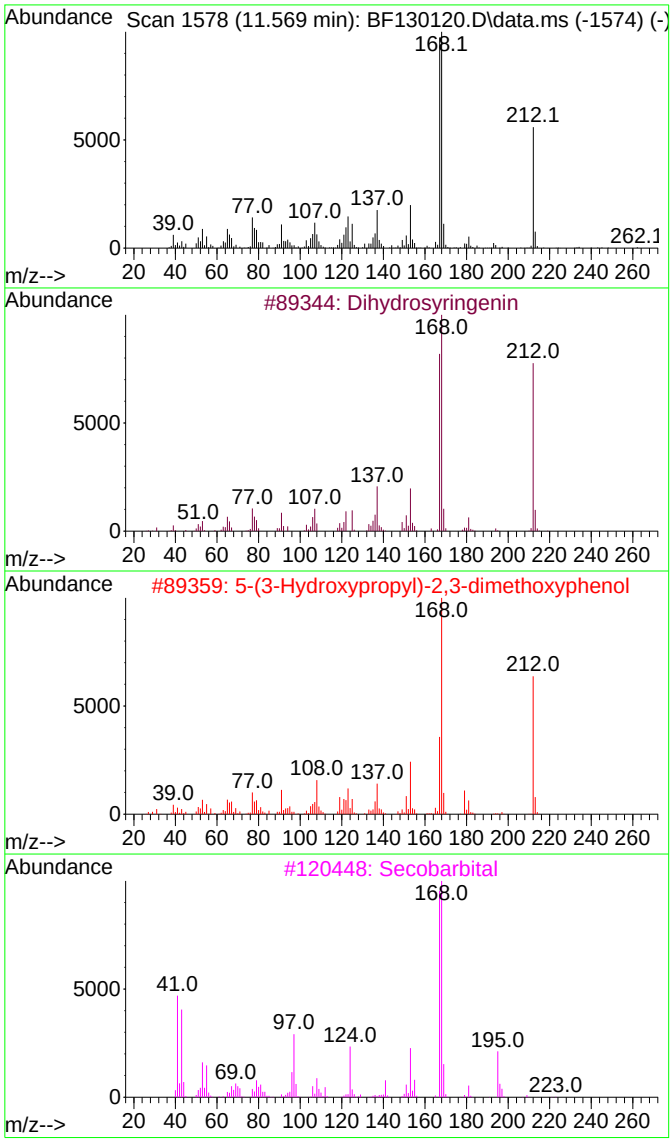
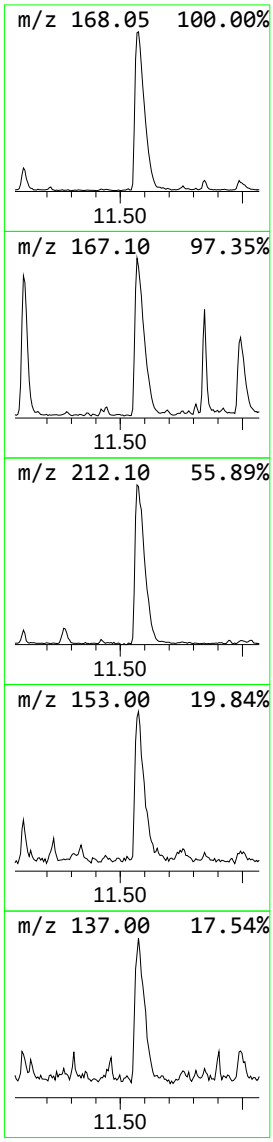
Peak Number 11 Dihydrosyringenin Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.569	12.87 ng	1072350	Phenanthrene-d10	11.216

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dihydrosyringenin	212	C11H16O4	020736-25-8	98
2	5-(3-Hydroxypropyl)-2,3-dimethox...	212	C11H16O4	063543-12-4	86
3	Secobarbital	238	C12H18N2O3	000076-73-3	50
4	Diphenylmethane	168	C13H12	000101-81-5	50
5	3,4-Dihydroxy-5-methoxybenzaldehyde	168	C8H8O4	003934-87-0	49





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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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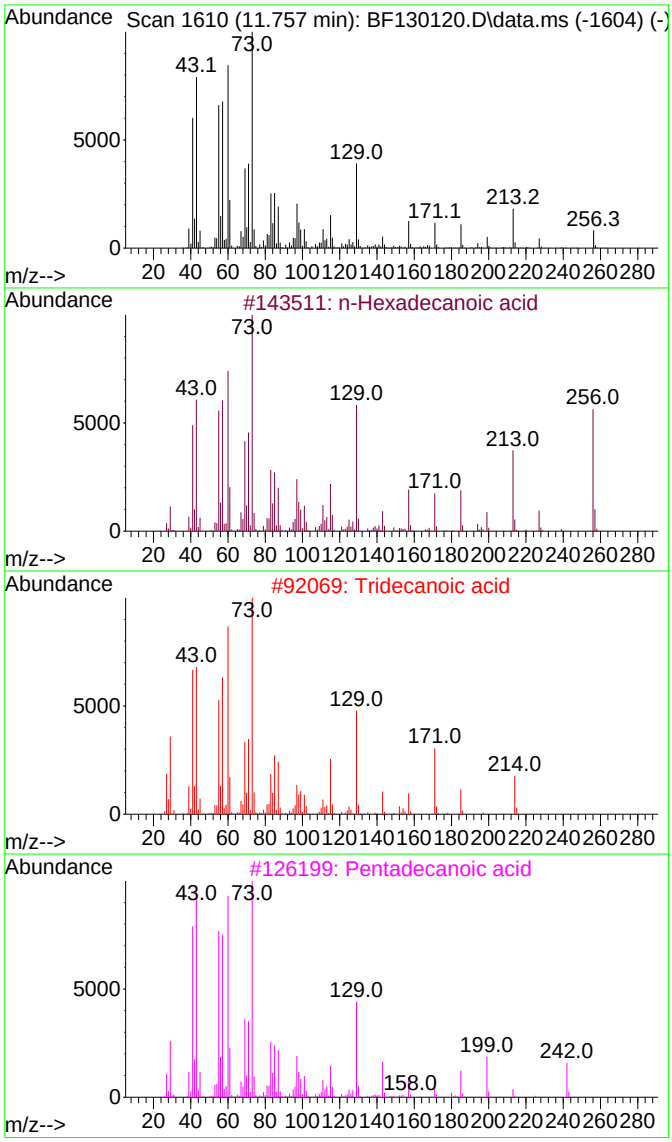
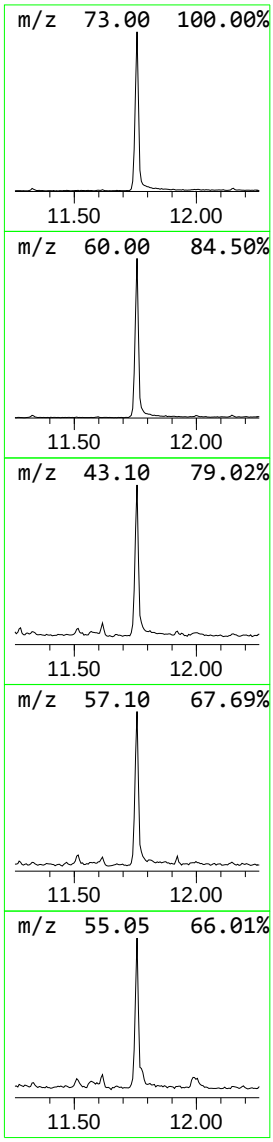
Peak Number 12 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.757	18.50 ng	1542290	Phenanthrene-d10	11.216

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	94
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
5	n-Decanoic acid	172	C10H20O2	000334-48-5	68





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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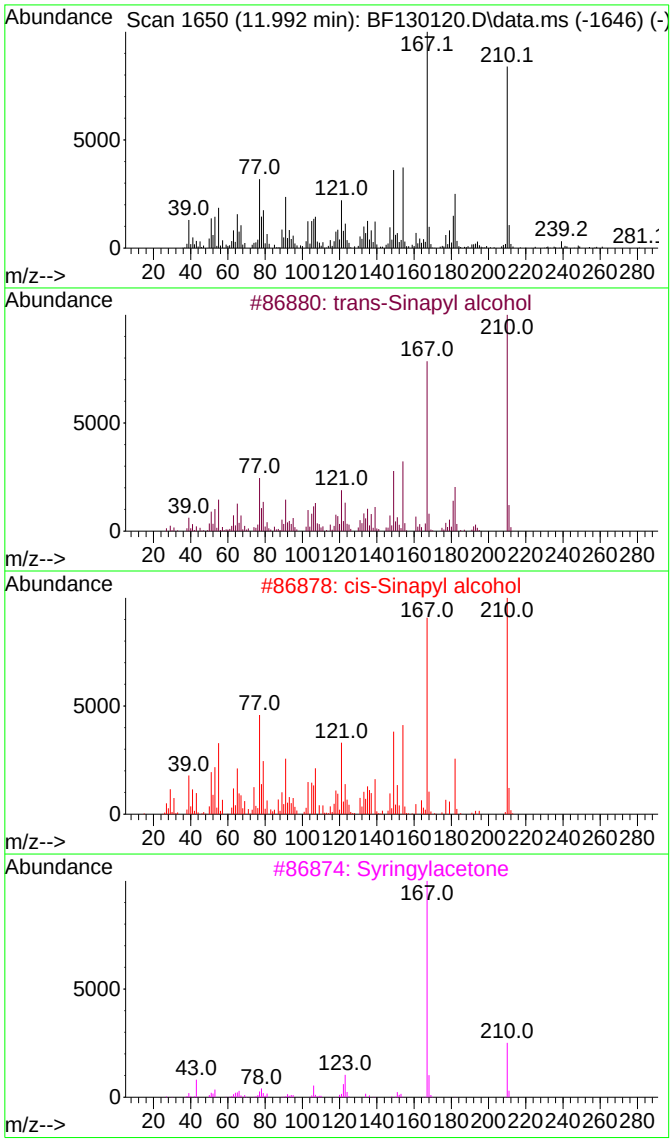
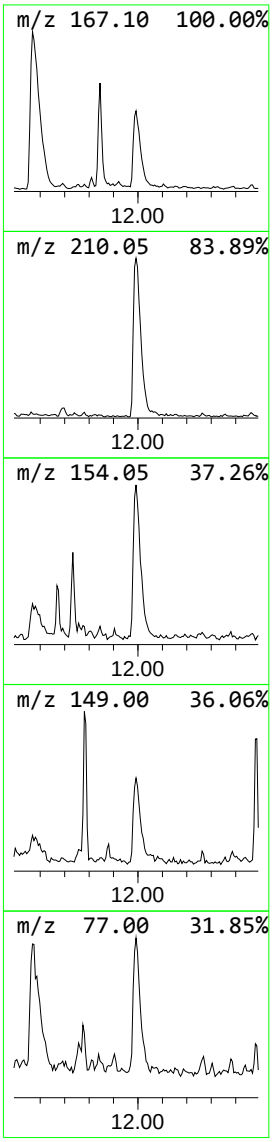
Peak Number 13 trans-Sinapyl alcohol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.992	8.19 ng	682752	Phenanthrene-d10	11.216

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-Sinapyl alcohol	210	C11H14O4	020675-96-1	96
2	cis-Sinapyl alcohol	210	C11H14O4	104330-63-4	94
3	Syringylacetone	210	C11H14O4	019037-58-2	64
4	4-Ethyl-2,6-dimethoxyphenol	182	C10H14O3	014059-92-8	60
5	1-(1-Hydroxybutyl)-2,5-dimethoxy...	210	C12H18O3	149083-03-4	58





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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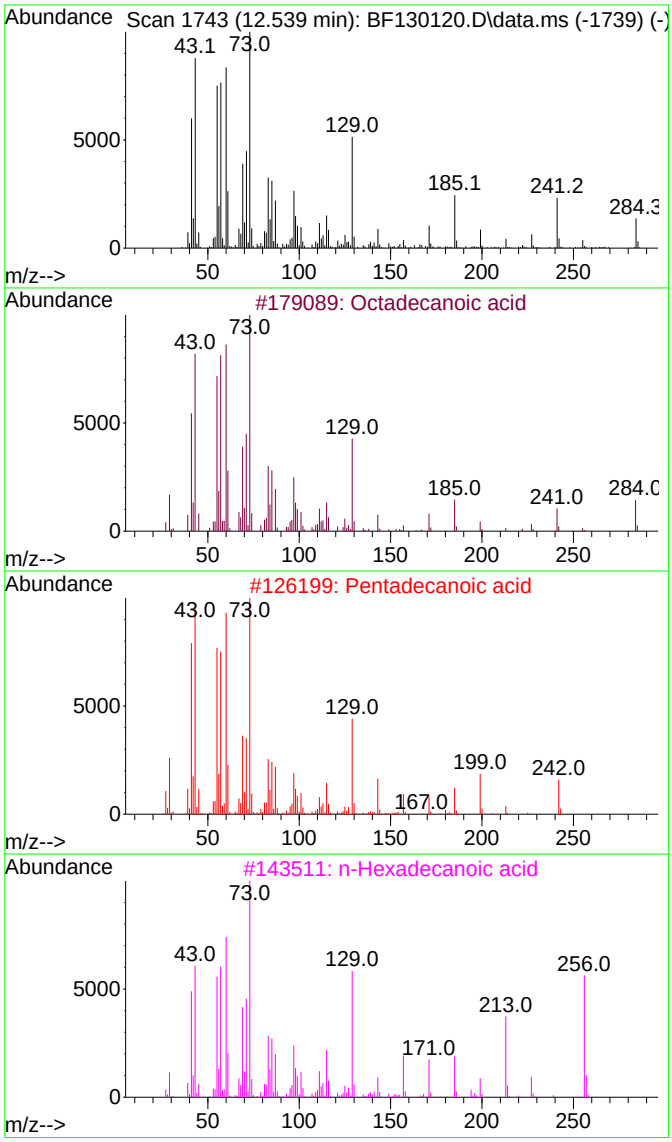
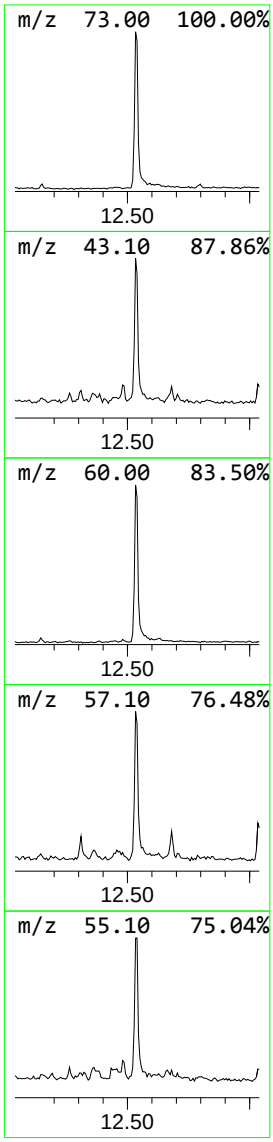
Peak Number 14 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.539	14.09 ng	728205	Chrysene-d12	13.839

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5	Undecane, 5-methyl-	170	C12H26	001632-70-8	25





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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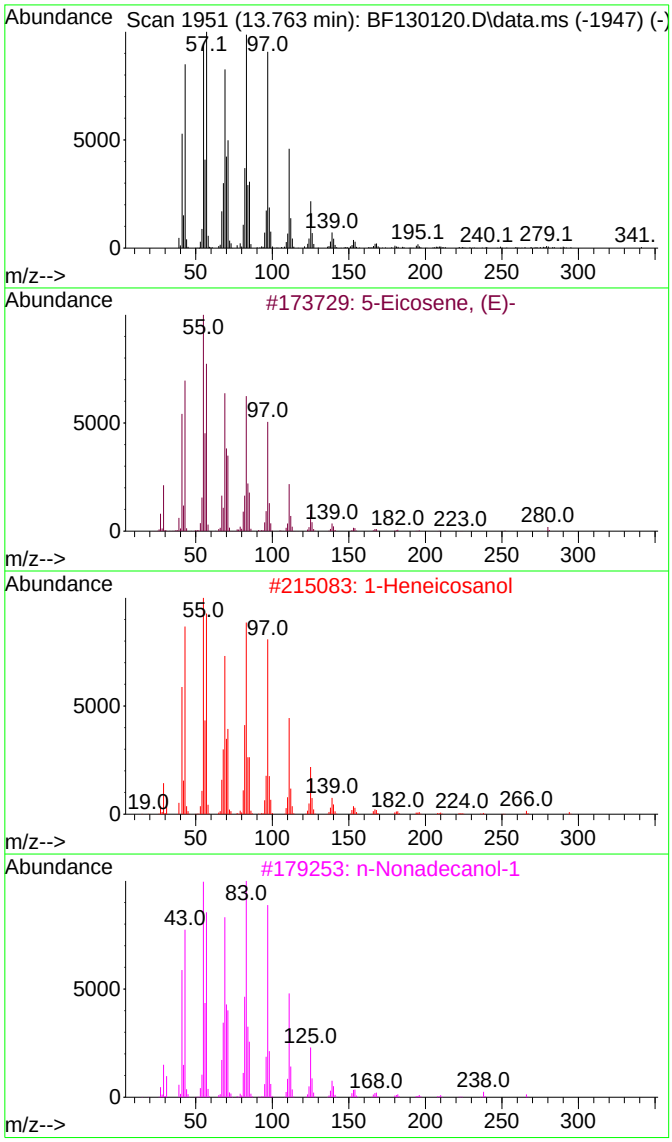
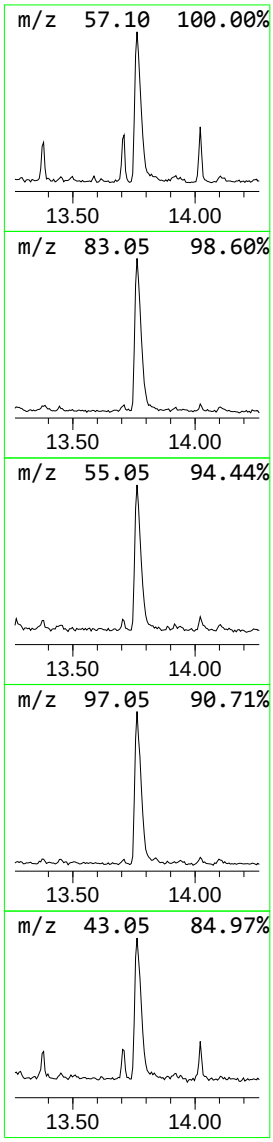
Peak Number 15 5-Eicosene, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.763	21.04 ng	1087640	Chrysene-d12	13.839

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94





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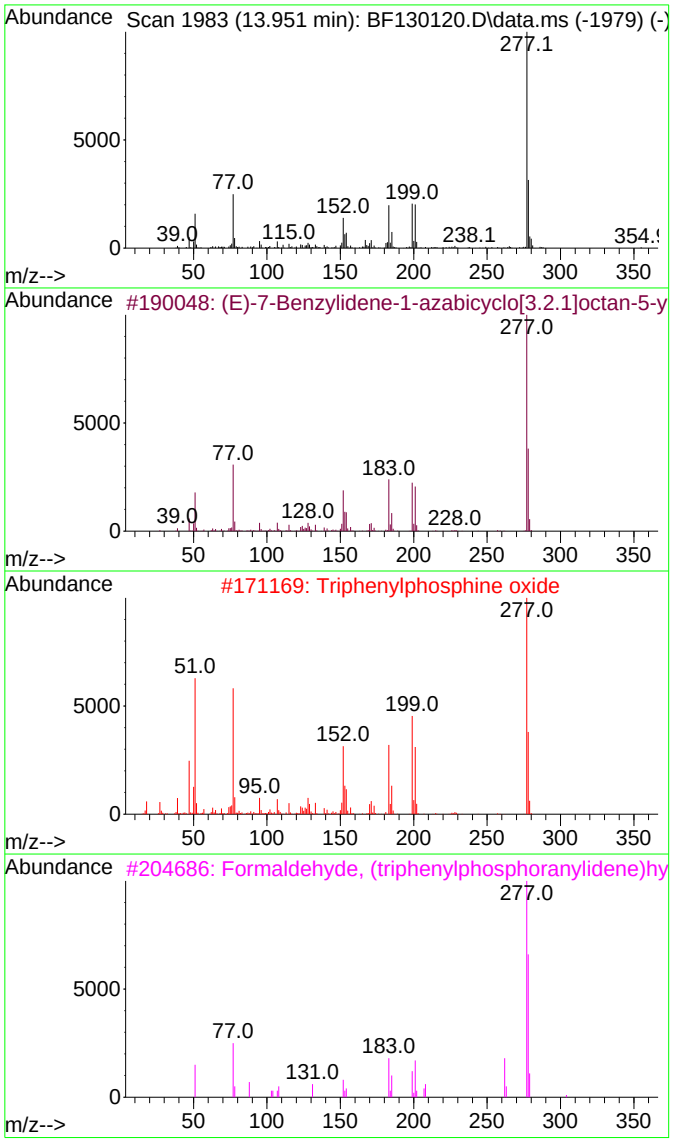
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

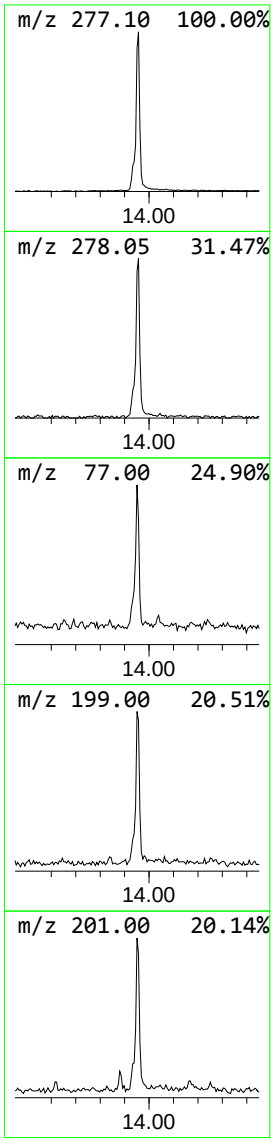
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 16 (E)-7-Benzylidene-1-azabicy... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.951	5.65 ng	291866	Chrysene-d12	13.839

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	91
2	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	90
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50
4	Benzoic acid, 2-(diphenylphosphi...	306	C19H15O2P	017261-28-8	36
5	(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	28





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Data File : BF130120.D
Acq On : 02 Sep 2022 19:58
Operator : CG\JU
Sample : N4455-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
KTS2-WC-L-MH-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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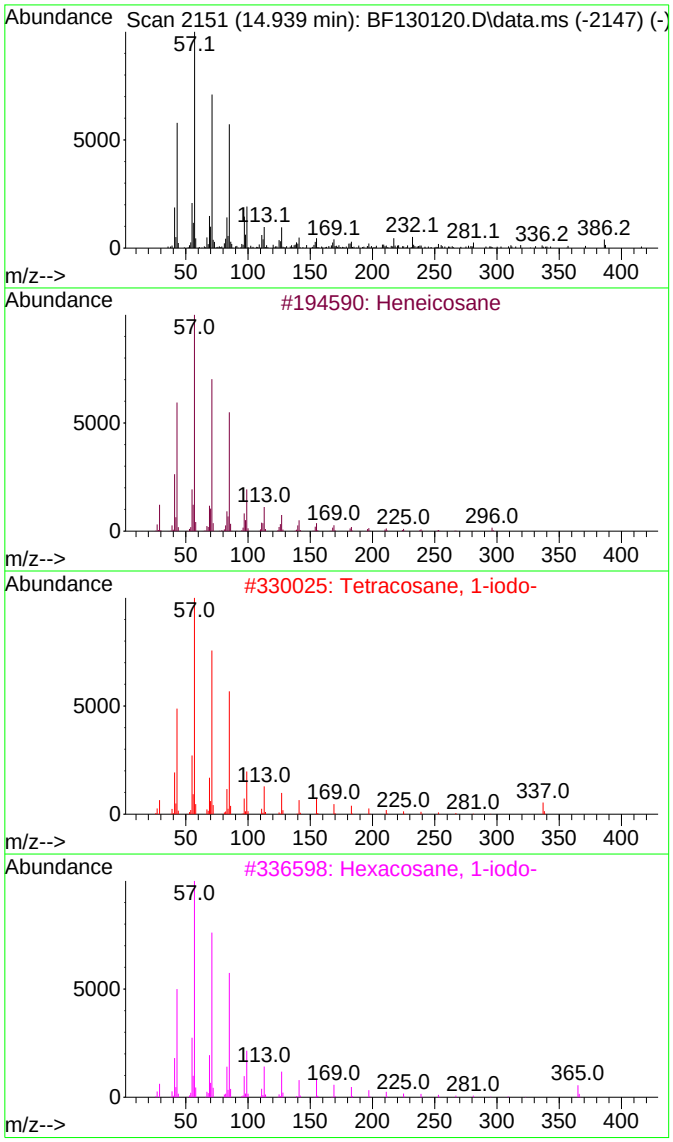
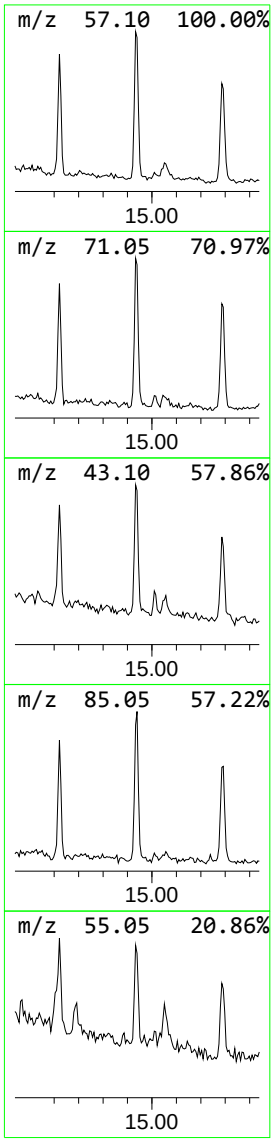
Peak Number 17 Heneicosane Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.939	4.14 ng	218815	Perylene-d12	15.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	90
3	Hexacosane, 1-iodo-	492	C26H53I	1000406-32-1	90
4	Tetracosane	338	C24H50	000646-31-1	90
5	Octacosane, 1-iodo-	520	C28H57I	1000406-32-2	90





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Data File : BF130120.D
Acq On : 02 Sep 2022 19:58
Operator : CG\JU
Sample : N4455-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
KTS2-WC-L-MH-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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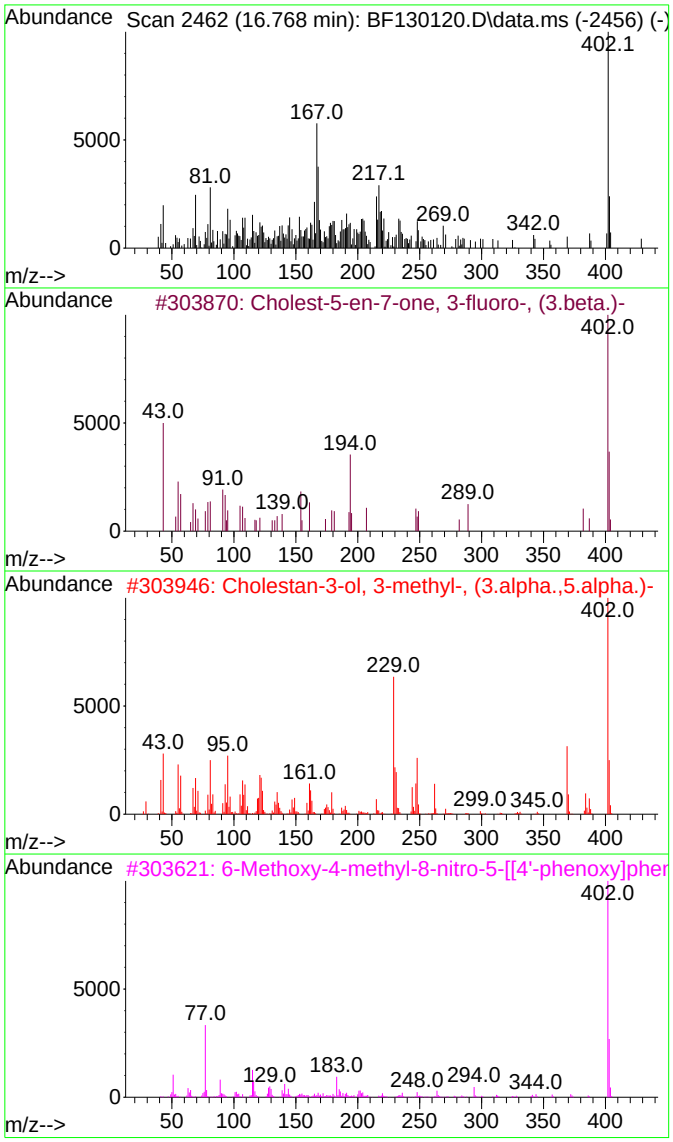
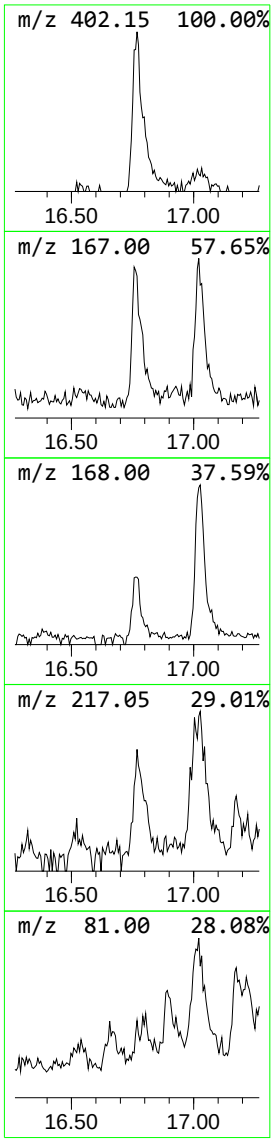
Peak Number 18 Cholest-5-en-7-one, 3-fluor... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.768	5.19 ng	274067	Perylene-d12	15.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholest-5-en-7-one, 3-fluoro-, (...	402	C27H43FO	031772-90-4	59
2	Cholestan-3-ol, 3-methyl-, (3.al...	402	C28H50O	001251-59-8	43
3	6-Methoxy-4-methyl-8-nitro-5-[[4...	402	C23H18N2O5	1000212-34-0	43
4	1,1'-Biphenyl, 4,4'-bis(4-propyl...	402	C30H42	085600-56-2	43
5	6-Methoxy-3-methyl-8-nitro-5-[[4...	402	C23H18N2O5	1000212-32-6	43





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Data File : BF130120.D
Acq On : 02 Sep 2022 19:58
Operator : CG\JU
Sample : N4455-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
KTS2-WC-L-MH-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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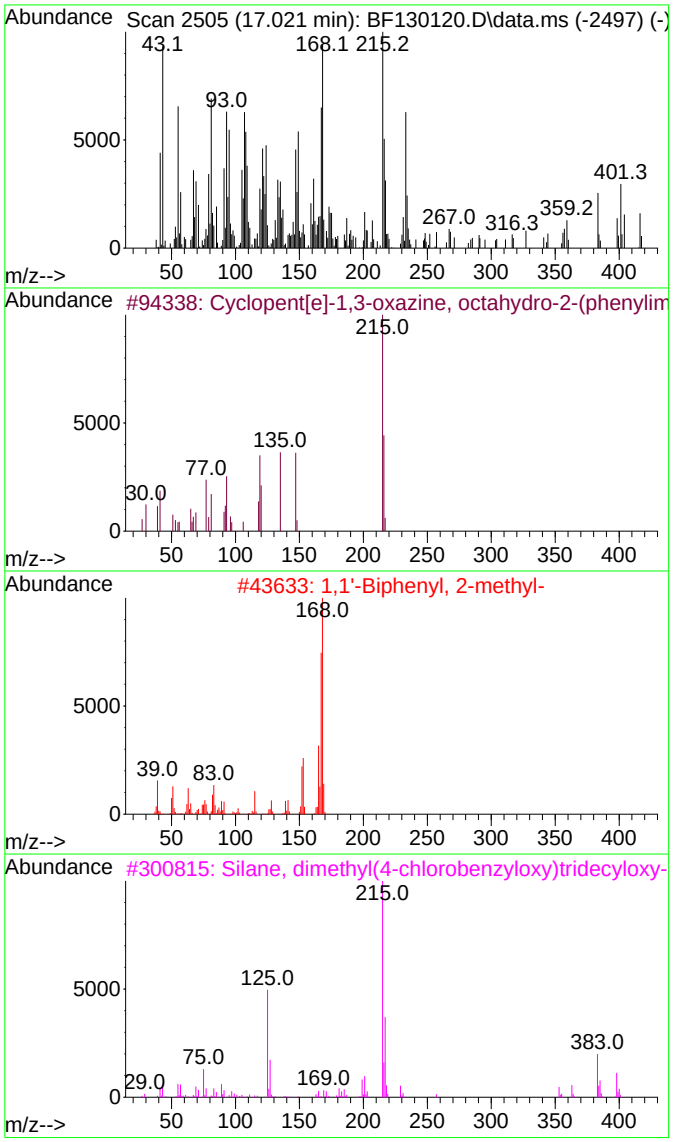
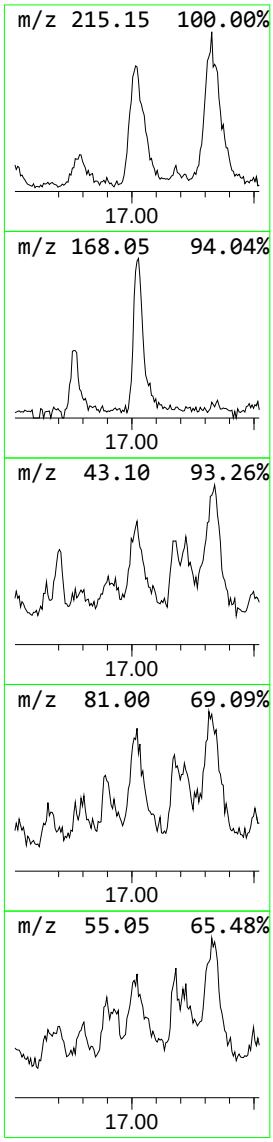
Peak Number 19 unknown17.021 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.021	8.73 ng	461626	Perylene-d12	15.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopent[e]-1,3-oxazine, octahy...	216	C13H16N2O	1000138-92-2	35
2	1,1'-Biphenyl, 2-methyl-	168	C13H12	000643-58-3	20
3	Silane, dimethyl(4-chlorobenzylo...	398	C22H39ClO2Si	1010347-00-1	20
4	Cholestane-3,6-diol, (3.beta.,5....	404	C27H48O2	041083-77-6	20
5	Diphenylmethane	168	C13H12	000101-81-5	20





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090222\
Data File : BF130120.D
Acq On : 02 Sep 2022 19:58
Operator : CG\JU
Sample : N4455-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
KTS2-WC-L-MH-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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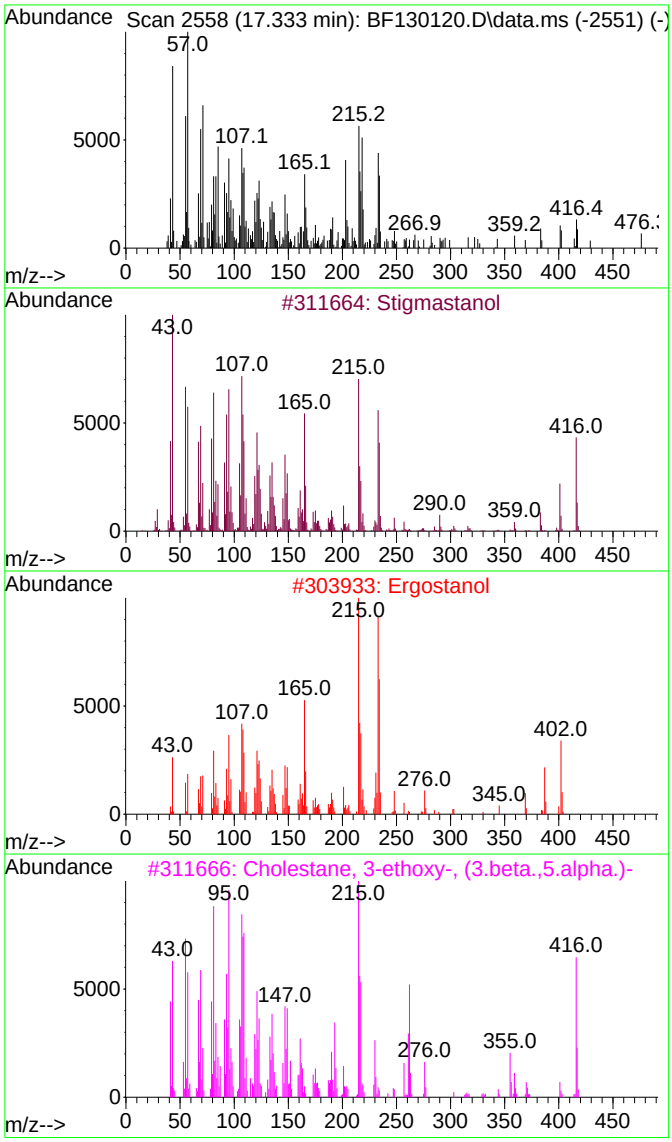
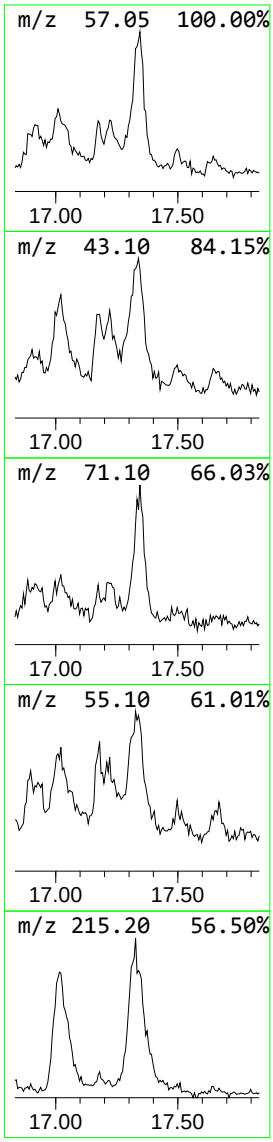
Peak Number 20 Stigmastanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.333	14.07 ng	743359	Perylene-d12	15.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Stigmastanol	416	C29H52O	019466-47-8	91
2	Ergostanol	402	C28H50O	006538-02-9	86
3	Cholestane, 3-ethoxy-, (3.beta.,...	416	C29H52O	002089-02-3	64
4	Cholestan-3-one, 4,4-dimethyl-, ...	414	C29H50O	002097-85-0	41
5	7-Oxabicyclo[4.1.0]heptane, 2,2,...	218	C15H22O	070038-20-9	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090222\
Data File : BF130120.D
Acq On : 02 Sep 2022 19:58
Operator : CG\JU
Sample : N4455-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
KTS2-WC-L-MH-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	4.898	5.5	ng	337622	1	6.704	1225800	20.0
2-Furanmethanol	5.081	12.8	ng	784016	1	6.704	1225800	20.0
trans-3-Methyl-...	8.769	35.5	ng	2884800	2	7.981	1627140	20.0
(3R,3aS,8aS)-3,...	9.392	6.2	ng	598491	3	9.733	1931690	20.0
2-Propanone, 1-...	9.863	7.5	ng	726053	3	9.733	1931690	20.0
Phenol, 2,6-dim...	10.192	6.1	ng	591367	3	9.733	1931690	20.0
Ethanone, 1-(4-...	10.822	4.3	ng	358409	4	11.216	1666950	20.0
4-(1-Hydroxyall...	10.945	7.1	ng	590246	4	11.216	1666950	20.0
Syringylacetone	10.969	16.8	ng	1400200	4	11.216	1666950	20.0
3,5-Dimethoxy-4...	11.104	6.4	ng	536046	4	11.216	1666950	20.0
Dihydrosyringenin	11.569	12.9	ng	1072350	4	11.216	1666950	20.0
n-Hexadecanoic ...	11.757	18.5	ng	1542290	4	11.216	1666950	20.0
trans-Sinapyl a...	11.992	8.2	ng	682752	4	11.216	1666950	20.0
Octadecanoic acid	12.539	14.1	ng	728205	5	13.839	1033730	20.0
5-Eicosene, (E)-	13.763	21.0	ng	1087640	5	13.839	1033730	20.0
(E)-7-Benzylide...	13.951	5.7	ng	291866	5	13.839	1033730	20.0
Heneicosane	14.939	4.1	ng	218815	6	15.245	1056990	20.0
Cholest-5-en-7-...	16.768	5.2	ng	274067	6	15.245	1056990	20.0
unknown17.021	17.021	8.7	ng	461626	6	15.245	1056990	20.0
Stigmastanol	17.333	14.1	ng	743359	6	15.245	1056990	20.0