

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090121\
 Data File : BF125311.D
 Acq On : 1 Sep 2021 17:39
 Operator : JU/CG
 Sample : M3616-01 2X
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CL-01-083121

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-BF081821.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125311.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.145	5	10	16	rVB	543454	671859	23.81%	2.485%
2	5.522	579	584	587	rBV	2517254	2388241	84.65%	8.832%
3	6.528	751	755	759	rBV	2425842	2391255	84.75%	8.843%
4	6.904	816	819	823	rBV	1519436	1177876	41.75%	4.356%
5	7.086	847	850	852	rBV	46053	38737	1.37%	0.143%
6	7.469	911	915	918	rBV	1724818	1528159	54.16%	5.651%
7	8.092	1018	1021	1031	rBV	51285	126685	4.49%	0.468%
8	8.192	1034	1038	1040	rBV	1769343	1580229	56.01%	5.844%
9	9.263	1216	1220	1223	rBV	3549180	2821432	100.00%	10.434%
10	9.339	1230	1233	1236	rVB	57603	47003	1.67%	0.174%
11	9.374	1236	1239	1243	rBV2	45400	49534	1.76%	0.183%
12	9.651	1283	1286	1290	rBV2	227219	208155	7.38%	0.770%
13	9.710	1294	1296	1299	rVV3	41501	41308	1.46%	0.153%
14	9.810	1307	1313	1315	rBV2	155621	184853	6.55%	0.684%
15	9.857	1318	1321	1325	rVV	228455	209413	7.42%	0.774%
16	9.892	1325	1327	1329	rVV2	42915	43192	1.53%	0.160%
17	9.945	1329	1336	1339	rVV	2246239	1951441	69.16%	7.217%
18	9.980	1339	1342	1347	rVV5	74408	127293	4.51%	0.471%
19	10.051	1351	1354	1358	rBV5	31754	60363	2.14%	0.223%
20	10.263	1387	1390	1391	rBV2	63355	57411	2.03%	0.212%
21	10.280	1391	1393	1396	rVV4	72260	60061	2.13%	0.222%
22	10.315	1396	1399	1401	rVB3	56569	56744	2.01%	0.210%
23	10.351	1401	1405	1409	rBV3	208007	191529	6.79%	0.708%
24	10.404	1411	1414	1416	rBV3	77214	83103	2.95%	0.307%
25	10.492	1426	1429	1431	rBV3	63247	71358	2.53%	0.264%
26	10.733	1466	1470	1473	rBV	2007884	1722793	61.06%	6.371%
27	10.851	1487	1490	1493	rBV	257958	243468	8.63%	0.900%
28	11.174	1542	1545	1546	rBV3	91421	86155	3.05%	0.319%
29	11.433	1586	1589	1592	rBV	2041862	1780537	63.11%	6.585%
30	11.457	1592	1593	1597	rVV	361446	225326	7.99%	0.833%
31	11.510	1600	1602	1604	rVV	77421	51715	1.83%	0.191%
32	11.951	1675	1677	1684	rVB5	223968	294778	10.45%	1.090%
33	12.651	1793	1796	1799	rVB	498193	447378	15.86%	1.654%
34	12.880	1832	1835	1840	rVB	494793	484101	17.16%	1.790%
35	13.015	1855	1858	1862	rVB	2153412	2052669	72.75%	7.591%
36	14.080	2034	2039	2041	rBV2	1297537	1408044	49.91%	5.207%

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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-BF081821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.103	2041	2043	2045	rVB	237691	173195	6.14%	0.640%
38	15.133	2215	2218	2221	rBV	238446	316892	11.23%	1.172%
39	15.515	2280	2283	2289	rVB	180996	257492	9.13%	0.952%
40	15.580	2290	2294	2305	rVB	897951	1328994	47.10%	4.915%

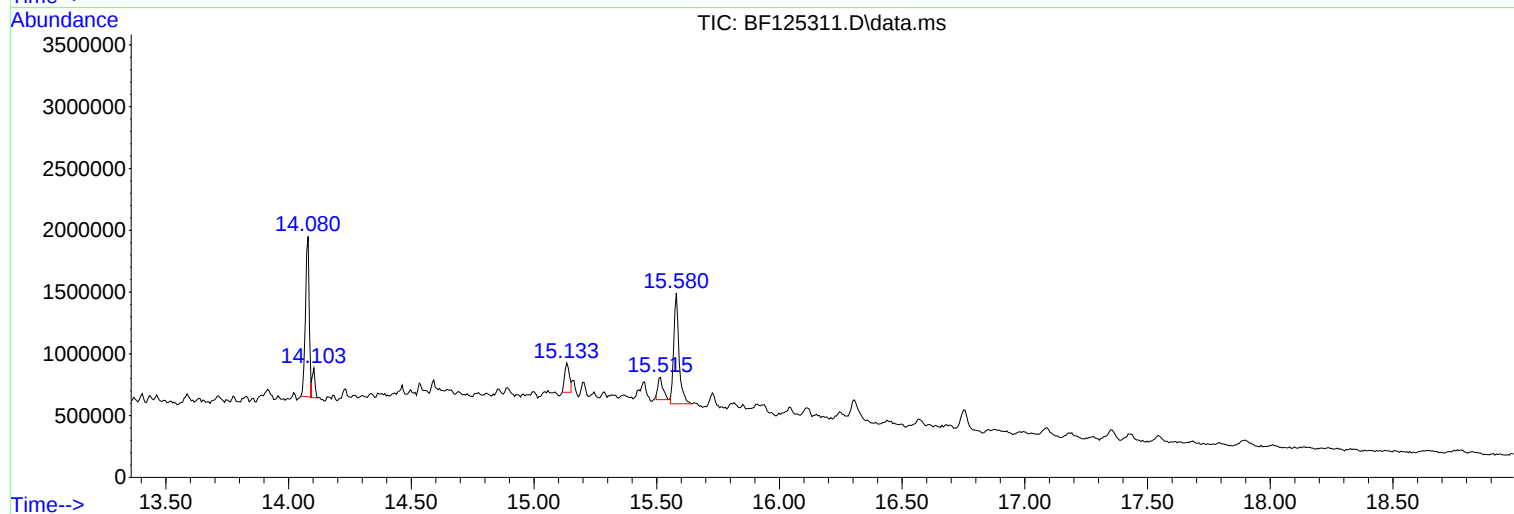
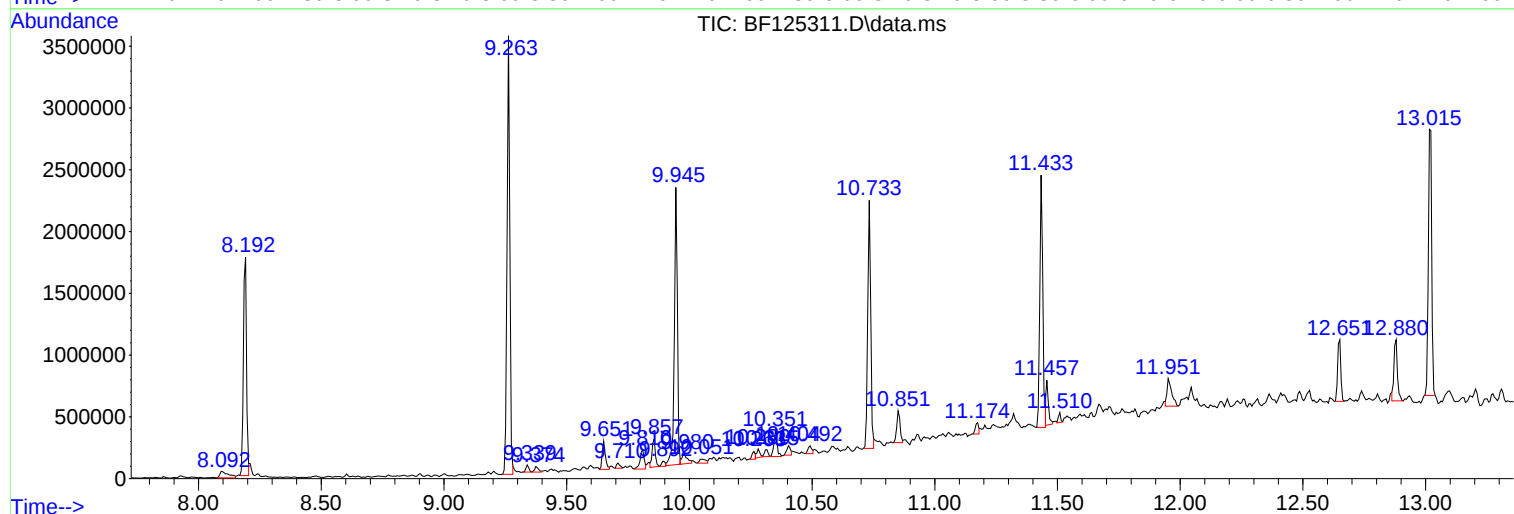
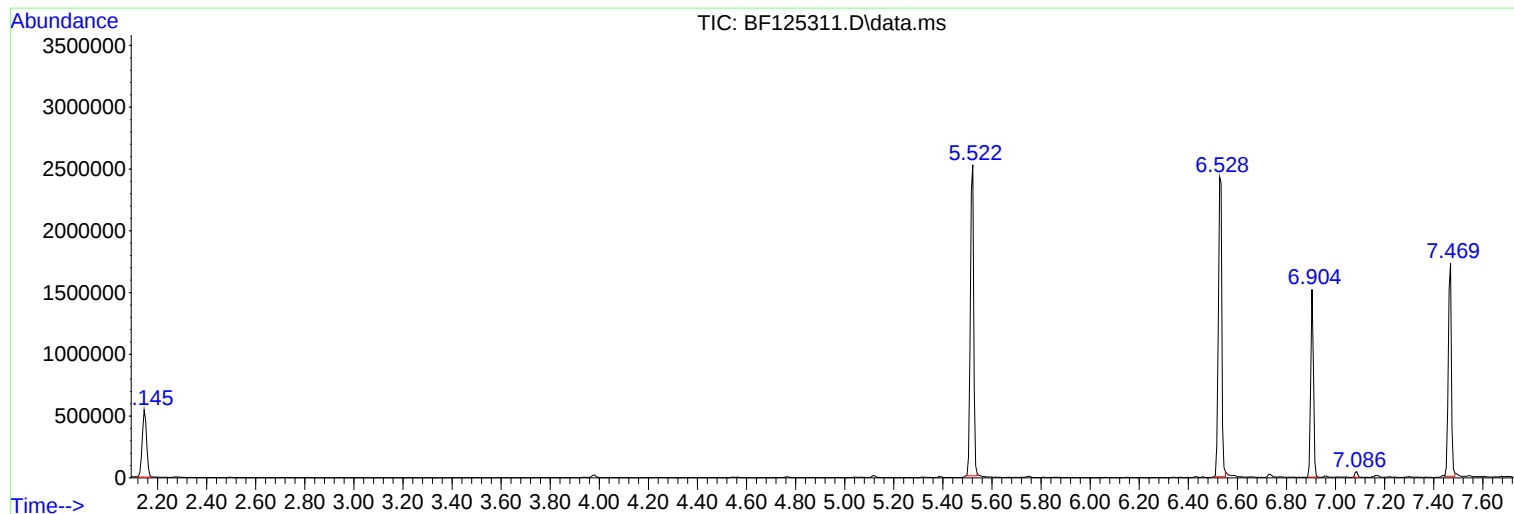
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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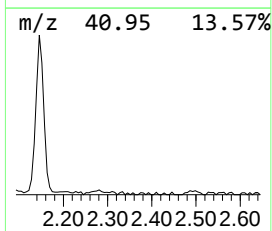
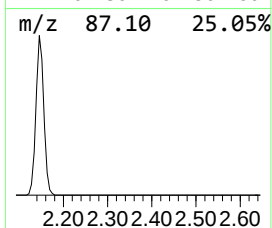
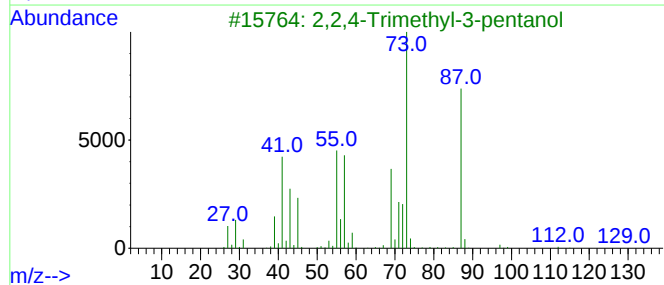
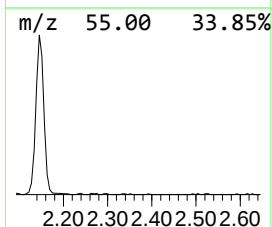
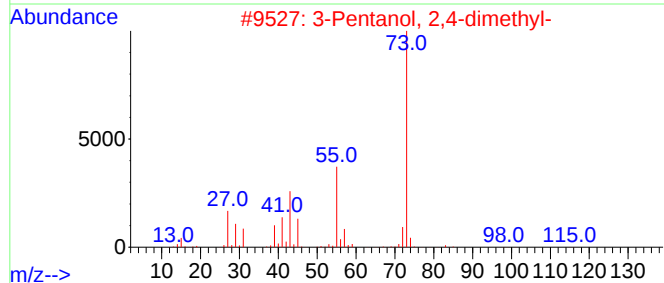
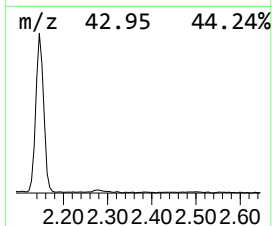
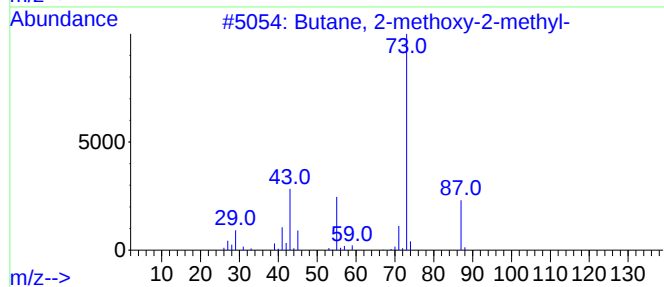
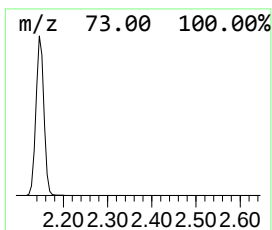
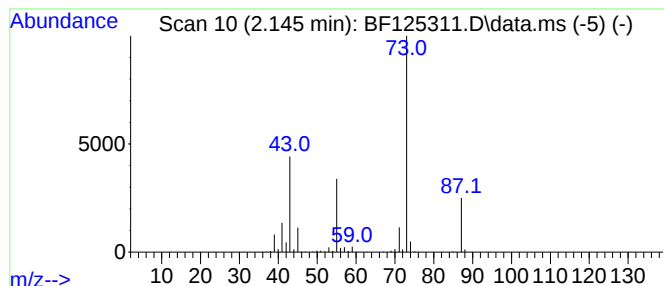
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.145	11.41 ng	671859	1,4-Dichlorobenzene-d4	6.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23



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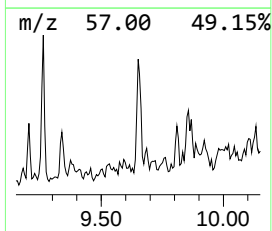
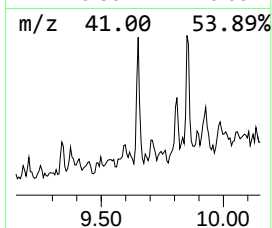
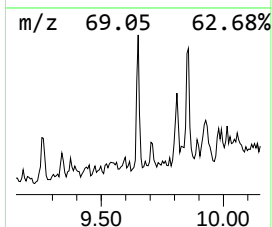
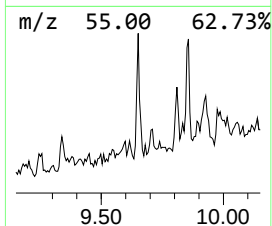
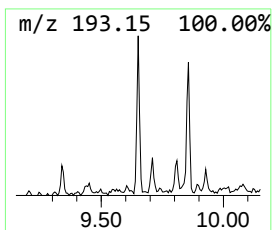
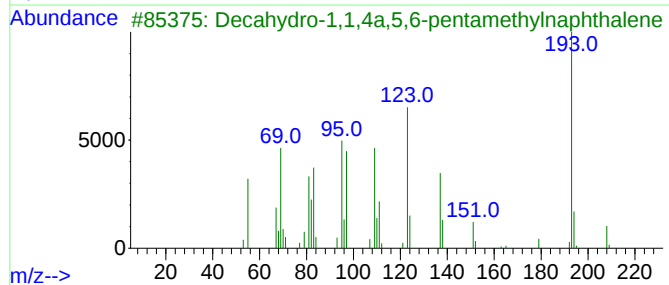
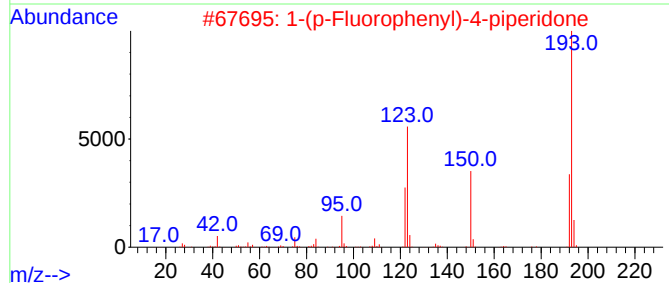
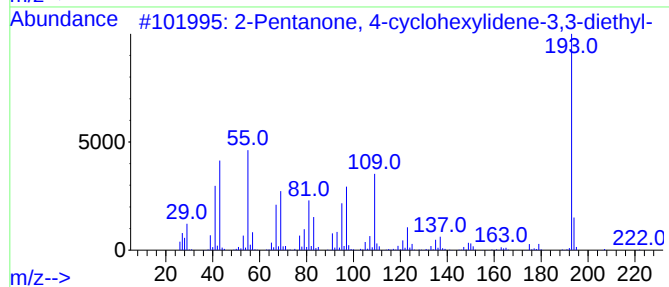
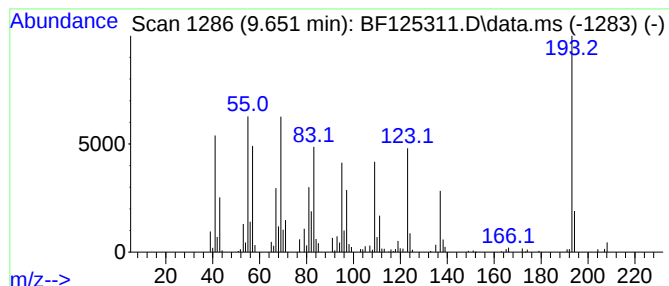
Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-cyclohexylidene-3,3-diethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
9.651	2.13 ng	208155	Acenaphthene-d10		9.945	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-cyclohexylidene-3...		222	C15H26O	313253-65-5	47
2	1-(p-Fluorophenyl)-4-piperidone		193	C11H12FNO	1000238-56-7	38
3	Decahydro-1,1,4a,5,6-pentamethyl...		208	C15H28	080655-44-3	38
4	Iminostilbene		193	C14H11N	000256-96-2	37
5	Acridine, 9-methyl-		193	C14H11N	000611-64-3	14



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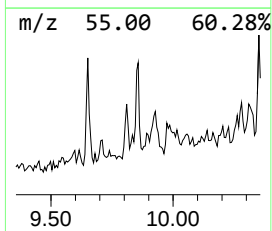
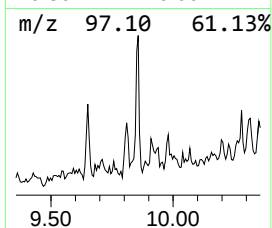
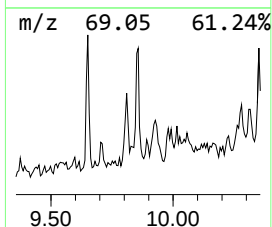
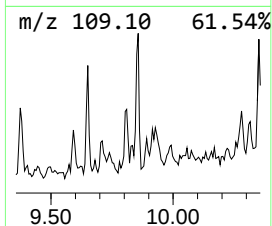
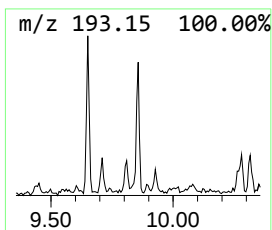
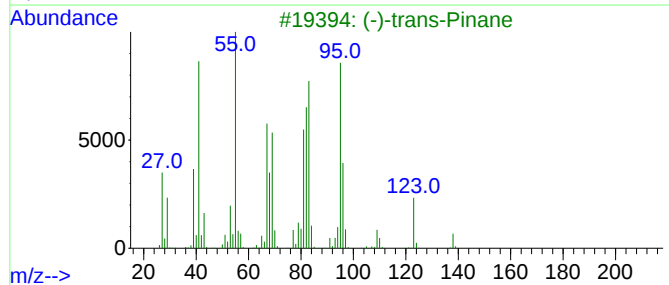
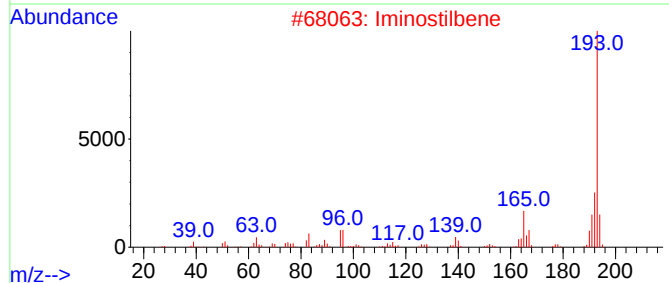
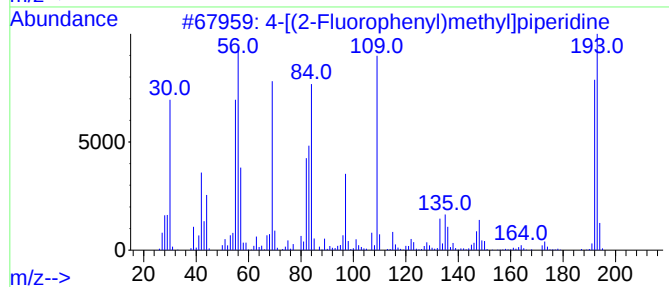
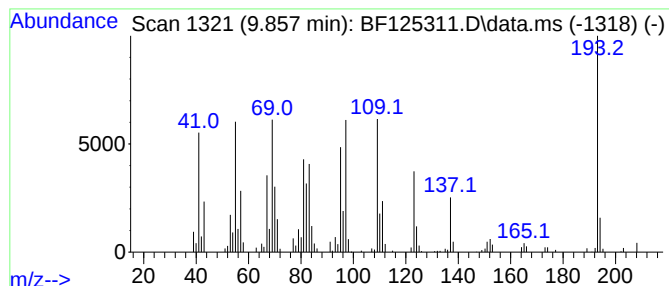
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown9.857 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.857	2.15 ng	209413	Acenaphthene-d10	9.945

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-[(2-Fluorophenyl)methyl]piperi...	193	C12H16FN	194288-97-6	43		
2	Iminostilbene	193	C14H11N	000256-96-2	27		
3	(-)-trans-Pinane	138	C10H18	033626-25-4	25		
4	Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	000473-55-2	25		
5	Cyclohexane, 1-(cyclohexylmethyl)...	194	C14H26	054823-96-0	18		



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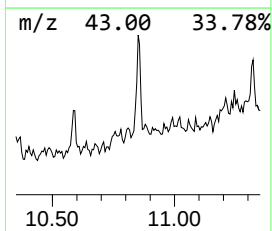
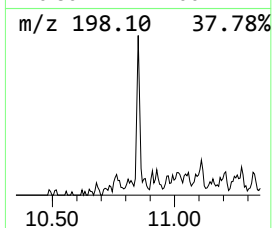
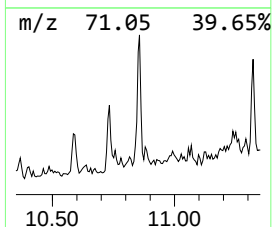
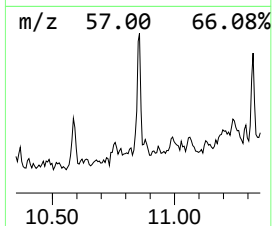
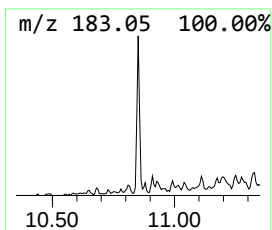
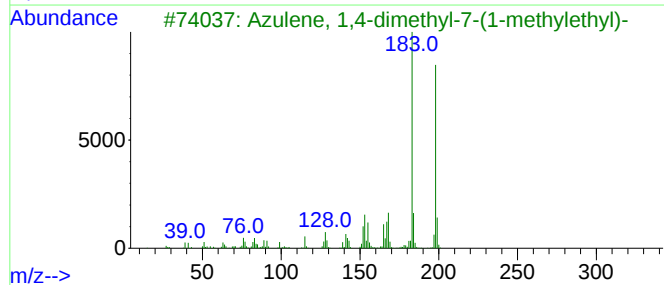
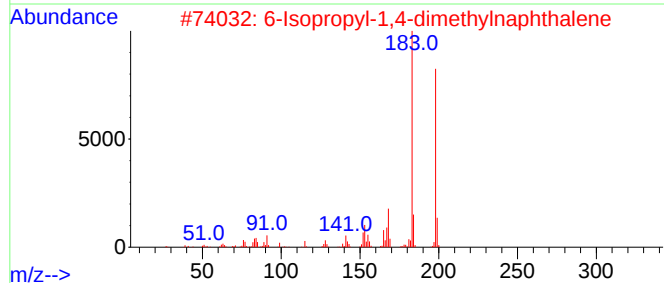
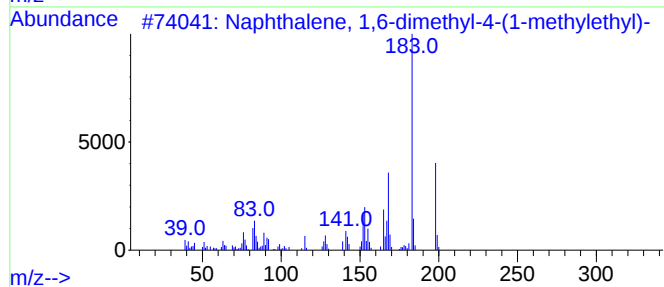
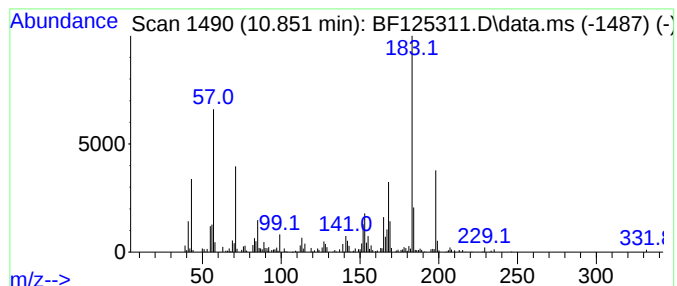
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Naphthalene, 1,6-dimethyl-4... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.851	2.73 ng	243468	Phenanthrene-d10	11.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,6-dimethyl-4-(1-m...	198	C15H18	000483-78-3	94
2			6-Isopropyl-1,4-dimethylnaphthalene	198	C15H18	000489-77-0	76
3			Azulene, 1,4-dimethyl-7-(1-methy...	198	C15H18	000489-84-9	70
4			Cyclopropane, 1,1,2,2-tetramethy...	198	C15H18	1000264-08-5	49
5			Ethanone, 1-[4-(methylsulfonyl)p...	198	C9H10O3S	010297-73-1	43



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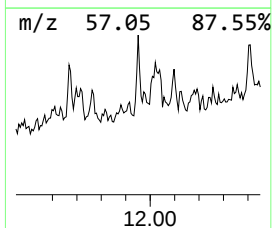
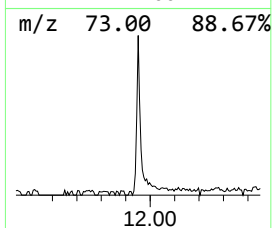
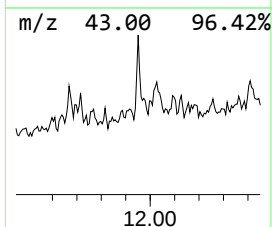
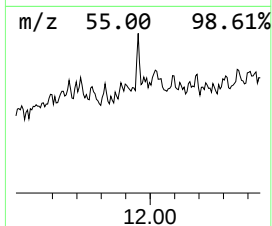
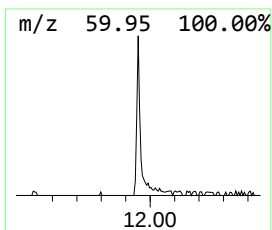
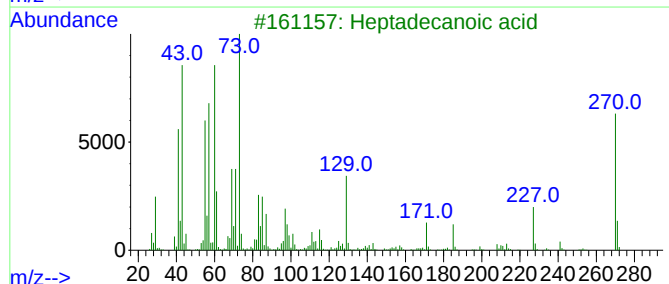
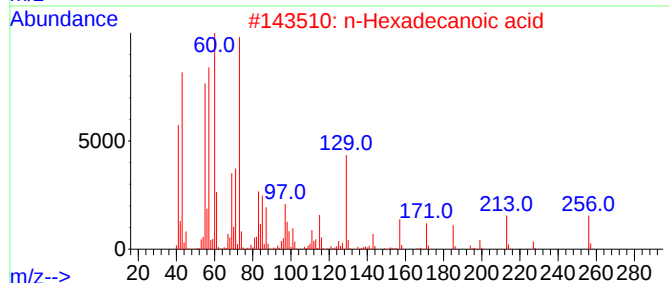
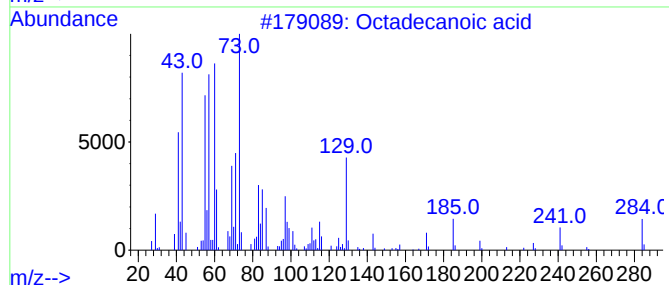
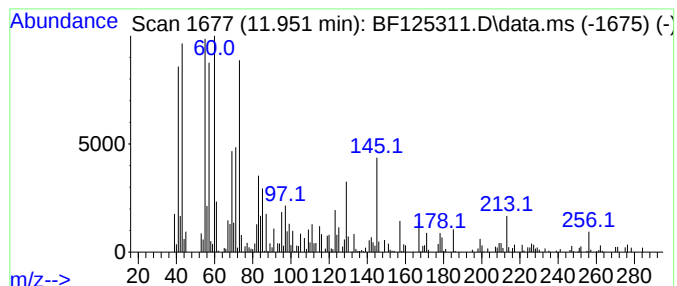
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.951	3.31 ng	294778	Phenanthrene-d10	11.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	93
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	92
3			Heptadecanoic acid	270	C17H34O2	000506-12-7	86
4			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	70
5			Estra-1,3,5(10)-trien-17.β-ol	256	C18H24O	002529-64-8	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090121\
Data File : BF125311.D
Acq On : 1 Sep 2021 17:39
Operator : JU/CG
Sample : M3616-01 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CL-01-083121

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.145	11.4	ng	671859	1	6.904	1177880	20.0
2-Pentanone, 4-...	9.651	2.1	ng	208155	3	9.945	1951440	20.0
unknown9.857	9.857	2.1	ng	209413	3	9.945	1951440	20.0
Naphthalene, 1,...	10.851	2.7	ng	243468	4	11.433	1780540	20.0
Octadecanoic acid	11.951	3.3	ng	294778	4	11.433	1780540	20.0