

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090921\
 Data File : BF125414.D
 Acq On : 9 Sep 2021 15:56
 Operator : JU/CG
 Sample : M3680-03 5X
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-SF-02-006-B

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: BF125414.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	6	10	19	rVB	190708	237174	20.39%	1.772%
2	3.957	313	318	323	rBV	14400	17595	1.51%	0.131%
3	5.092	508	511	515	rBV	17832	17454	1.50%	0.130%
4	5.498	577	580	591	rBV	746248	746535	64.19%	5.577%
5	6.510	749	752	763	rBV	829767	796666	68.50%	5.951%
6	6.886	812	816	819	rBV	1101317	972109	83.58%	7.262%
7	7.416	900	906	907	rBV4	16354	17206	1.48%	0.129%
8	7.445	907	911	920	rVV	554400	504442	43.37%	3.768%
9	7.528	920	925	929	rVB5	17814	25689	2.21%	0.192%
10	7.686	948	952	955	rVB3	17671	21458	1.84%	0.160%
11	7.804	970	972	976	rVB3	19239	17485	1.50%	0.131%
12	8.169	1030	1034	1037	rBV	1443163	1149501	98.83%	8.587%
13	8.222	1040	1043	1045	rVB3	35987	33577	2.89%	0.251%
14	8.251	1045	1048	1053	rVB5	14603	16279	1.40%	0.122%
15	8.457	1076	1083	1087	rBV7	20157	28354	2.44%	0.212%
16	8.551	1095	1099	1101	rVB4	13491	15808	1.36%	0.118%
17	8.580	1101	1104	1107	rBV	36309	33944	2.92%	0.254%
18	8.669	1116	1119	1122	rBV3	21138	19827	1.70%	0.148%
19	8.751	1131	1133	1137	rBV3	40152	36039	3.10%	0.269%
20	8.822	1142	1145	1149	rBV5	12185	18675	1.61%	0.140%
21	8.986	1171	1173	1176	rVB3	27229	19962	1.72%	0.149%
22	9.116	1191	1195	1196	rBV3	14282	18319	1.58%	0.137%
23	9.180	1204	1206	1209	rBV	54407	45419	3.91%	0.339%
24	9.239	1213	1216	1221	rBV	990355	833724	71.68%	6.228%
25	9.316	1226	1229	1232	rVB	58378	56369	4.85%	0.421%
26	9.392	1239	1242	1244	rVB3	29015	25693	2.21%	0.192%
27	9.504	1257	1261	1265	rBV4	20346	28467	2.45%	0.213%
28	9.557	1267	1270	1272	rBV3	14476	18035	1.55%	0.135%
29	9.580	1272	1274	1276	rVV2	36650	35022	3.01%	0.262%
30	9.639	1280	1284	1286	rBV2	73207	74825	6.43%	0.559%
31	9.698	1291	1294	1296	rVB3	21281	17202	1.48%	0.128%
32	9.786	1303	1309	1312	rBV5	33026	41779	3.59%	0.312%
33	9.845	1317	1319	1322	rVB	57237	44997	3.87%	0.336%
34	9.927	1327	1333	1336	rVV	1257480	1163083	100.00%	8.688%
35	9.957	1336	1338	1342	rVB2	31930	30013	2.58%	0.224%
36	10.027	1347	1350	1355	rBV4	21048	28646	2.46%	0.214%

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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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37	10.069	1355	1357	1360	rBV4	13213	19900	1.71%	0.149%
38	10.122	1362	1366	1370	rVV3	23676	45771	3.94%	0.342%
39	10.169	1370	1374	1378	rVV3	39880	39187	3.37%	0.293%
40	10.239	1383	1386	1388	rBV3	29618	27719	2.38%	0.207%
41	10.345	1398	1404	1407	rBV2	69813	75513	6.49%	0.564%
42	10.469	1420	1425	1428	rBV6	19495	39921	3.43%	0.298%
43	10.569	1438	1442	1447	rVB	62985	77389	6.65%	0.578%
44	10.710	1464	1466	1472	rBV	262951	236026	20.29%	1.763%
45	10.833	1482	1487	1494	rVB	131597	173413	14.91%	1.295%
46	11.045	1522	1523	1526	rVB3	23914	16243	1.40%	0.121%
47	11.269	1558	1561	1563	rBV	60386	51334	4.41%	0.383%
48	11.298	1563	1566	1573	rVB3	83865	95566	8.22%	0.714%
49	11.410	1582	1585	1588	rBV	1101818	1051966	90.45%	7.858%
50	11.433	1588	1589	1592	rVV	111872	95873	8.24%	0.716%
51	11.486	1596	1598	1601	rVB	25097	23318	2.00%	0.174%
52	11.651	1623	1626	1630	rBV3	32616	43854	3.77%	0.328%
53	11.698	1631	1634	1636	rVV	49052	47272	4.06%	0.353%
54	11.745	1640	1642	1648	rVB2	29822	35741	3.07%	0.267%
55	11.927	1669	1673	1679	rBV4	69668	127130	10.93%	0.950%
56	12.027	1687	1690	1692	rBV2	40304	43016	3.70%	0.321%
57	12.051	1692	1694	1697	rVB	31646	22373	1.92%	0.167%
58	12.104	1700	1703	1705	rBV	54994	48422	4.16%	0.362%
59	12.145	1708	1710	1713	rBV3	20679	17269	1.48%	0.129%
60	12.210	1719	1721	1723	rBV3	23807	19630	1.69%	0.147%
61	12.339	1741	1743	1745	rBV2	29570	27796	2.39%	0.208%
62	12.386	1749	1751	1754	rBV3	43834	44884	3.86%	0.335%
63	12.463	1761	1764	1766	rBV	62273	58076	4.99%	0.434%
64	12.492	1766	1769	1772	rVV3	78075	81116	6.97%	0.606%
65	12.521	1772	1774	1776	rVB3	27647	16538	1.42%	0.124%
66	12.551	1777	1779	1782	rBV4	26617	30034	2.58%	0.224%
67	12.627	1789	1792	1796	rBV	225731	197116	16.95%	1.472%
68	12.857	1828	1831	1837	rVB2	185712	201125	17.29%	1.502%
69	12.998	1851	1855	1858	rBV	770829	669019	57.52%	4.997%
70	13.221	1891	1893	1896	rBV2	62453	63973	5.50%	0.478%
71	13.563	1949	1951	1955	rBV2	95042	89049	7.66%	0.665%
72	13.892	2005	2007	2010	rVB	124289	86443	7.43%	0.646%
73	14.057	2031	2035	2038	rBV	947445	936348	80.51%	6.994%
74	14.210	2059	2061	2068	rVB	185049	196701	16.91%	1.469%
75	14.515	2111	2113	2115	rVB	189126	143756	12.36%	1.074%
76	15.557	2286	2290	2296	rVB2	584681	863896	74.28%	6.453%

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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

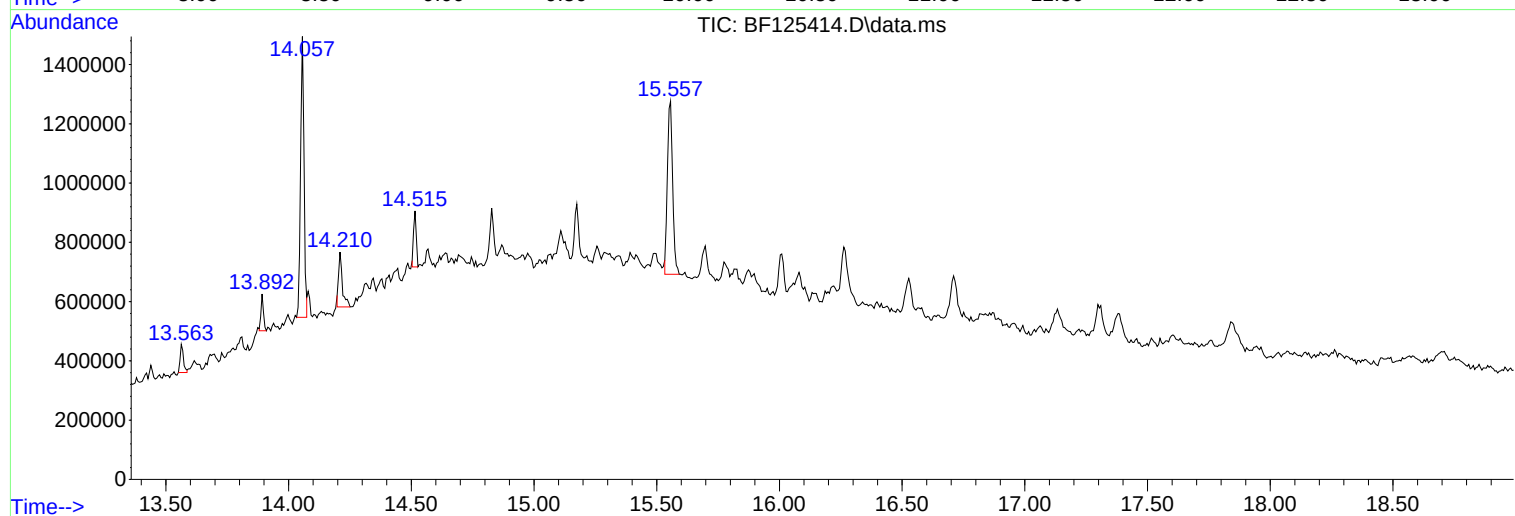
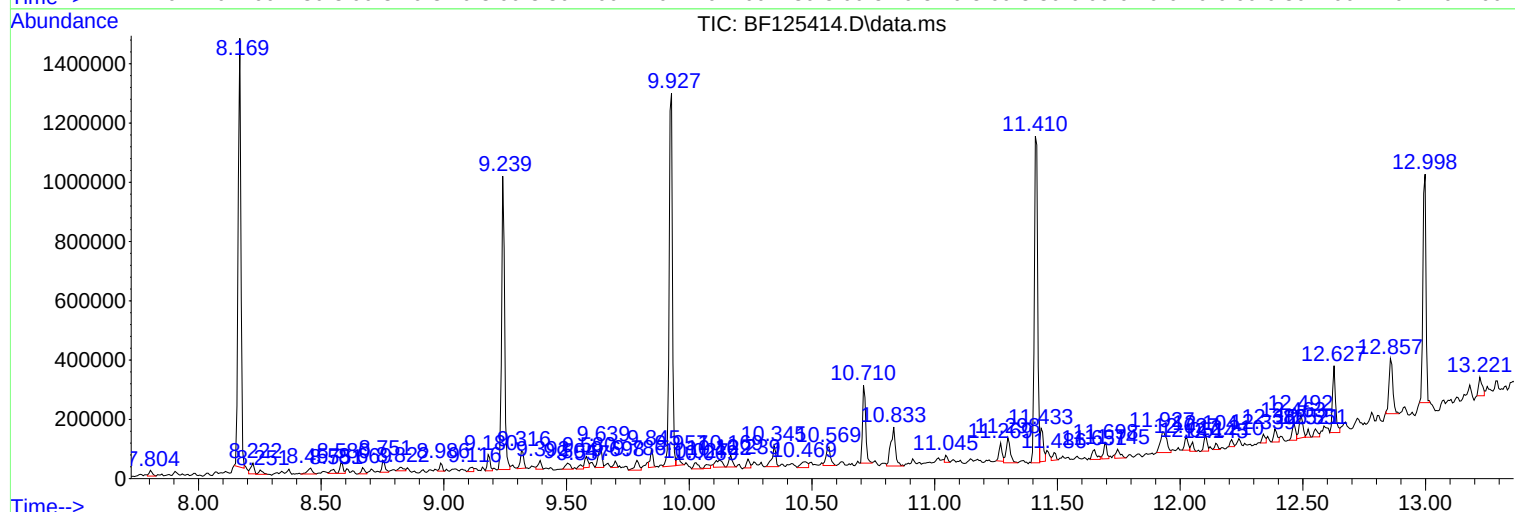
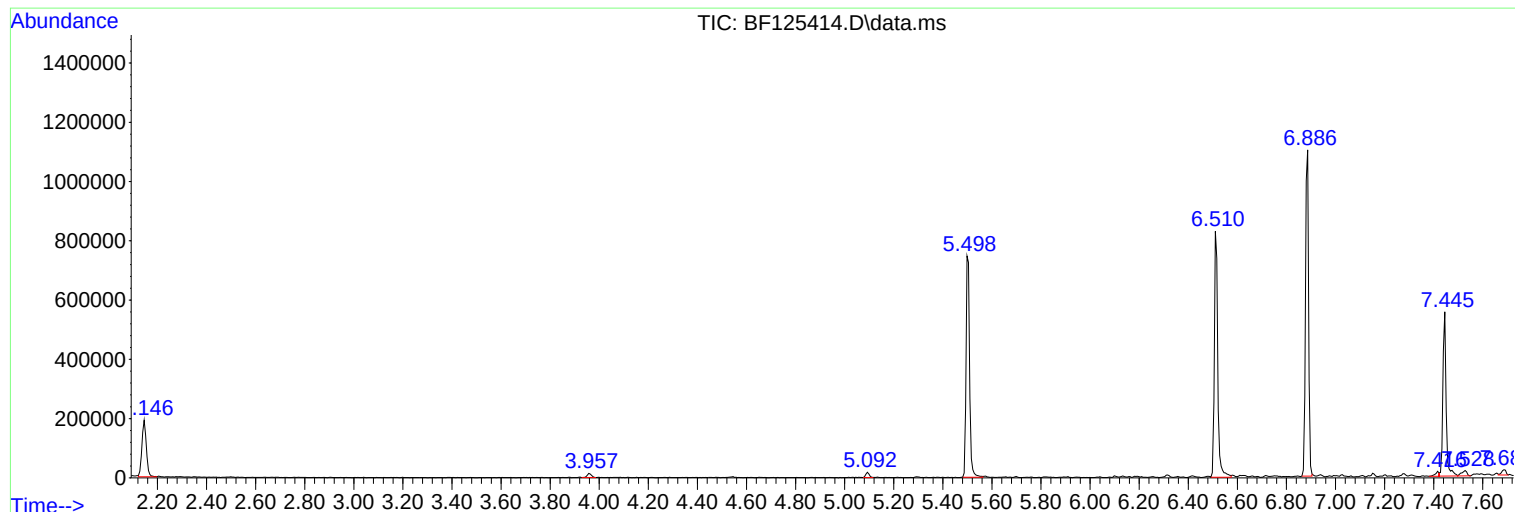
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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-SF-02-006-B

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090921\
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Sample : M3680-03 5X
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Instrument :
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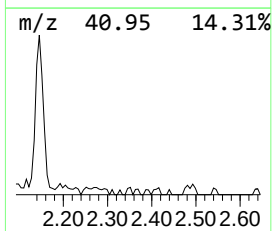
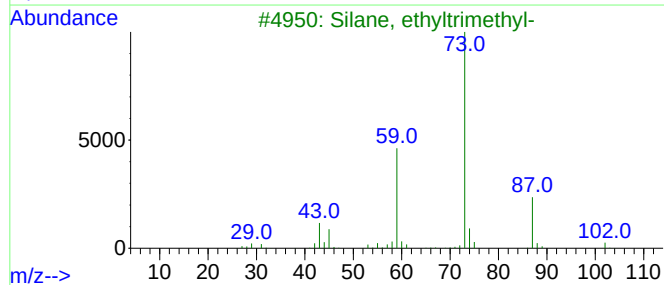
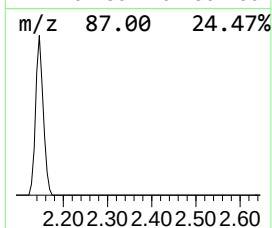
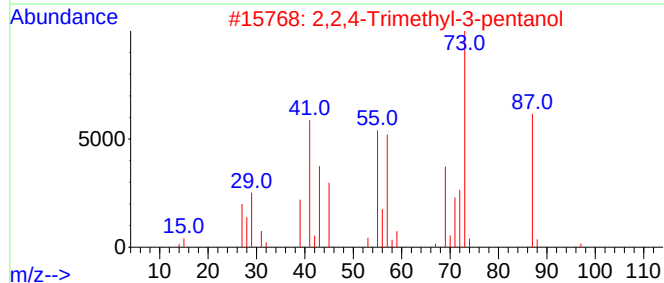
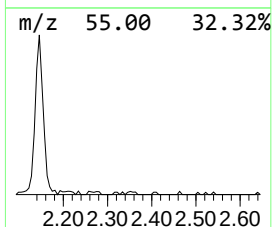
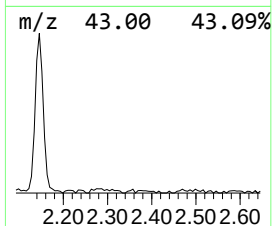
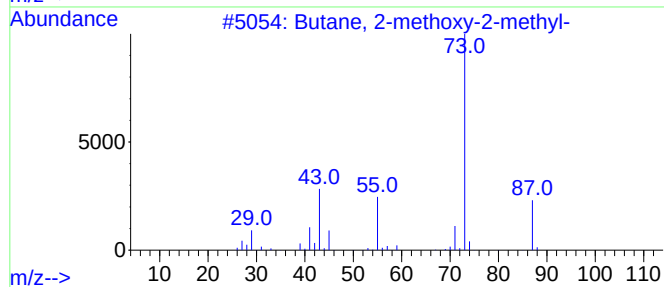
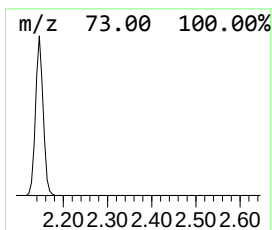
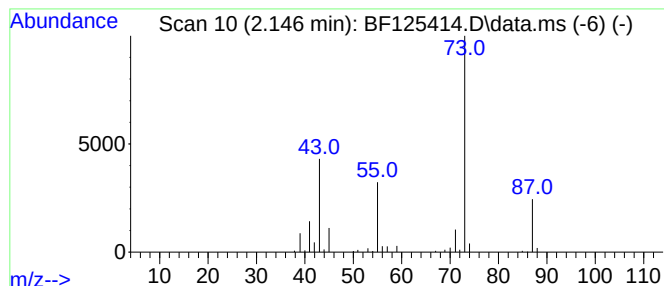
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.146	4.88 ng	237174	1,4-Dichlorobenzene-d4	6.886

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			Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	33
4			3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	25
5			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25



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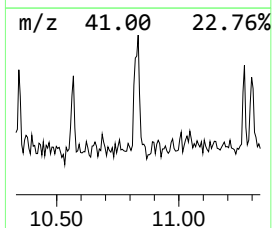
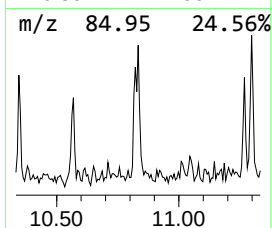
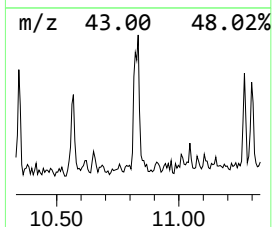
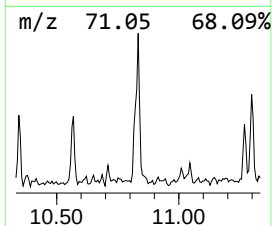
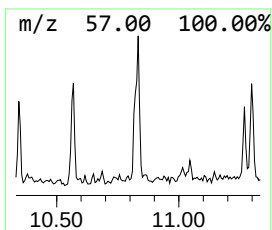
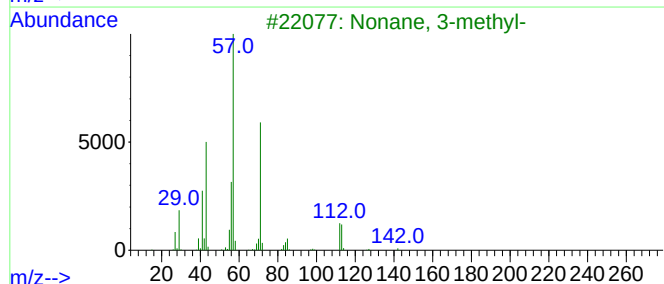
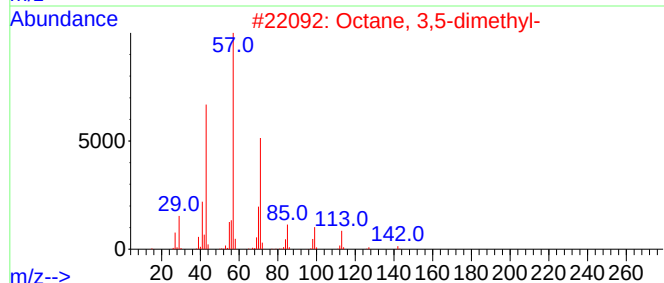
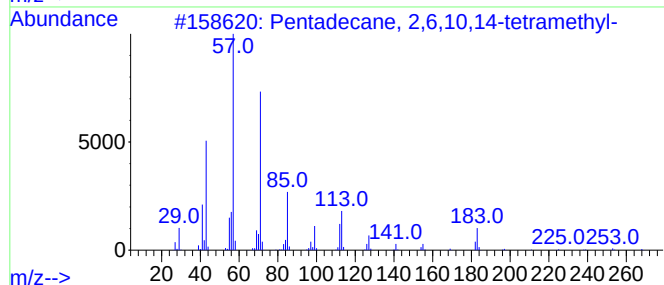
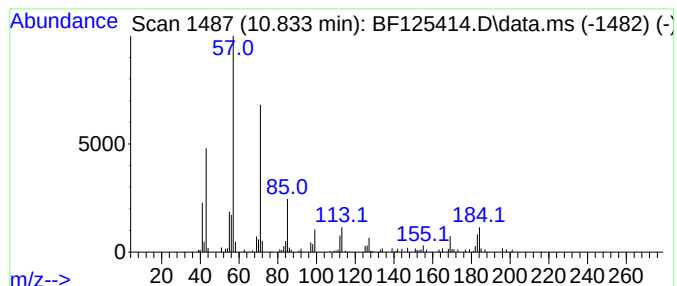
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Pentadecane, 2,6,10,14-tetr... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.833	3.30 ng	173413	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	64
2			Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	62
3			Nonane, 3-methyl-	142	C10H22	005911-04-6	53
4			Tridecane, 7-methyl-	198	C14H30	026730-14-3	52
5			Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	49



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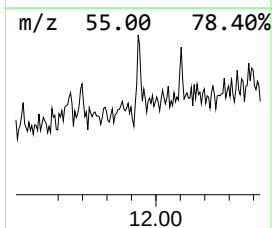
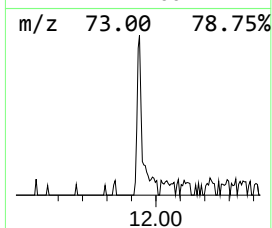
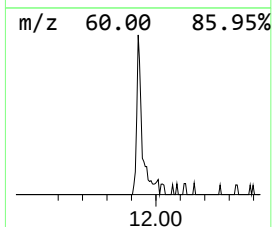
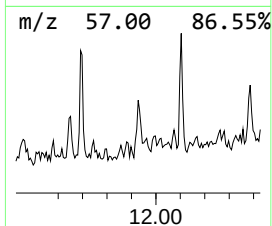
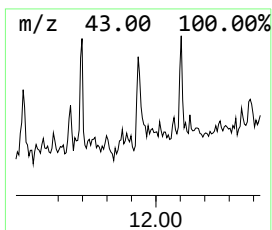
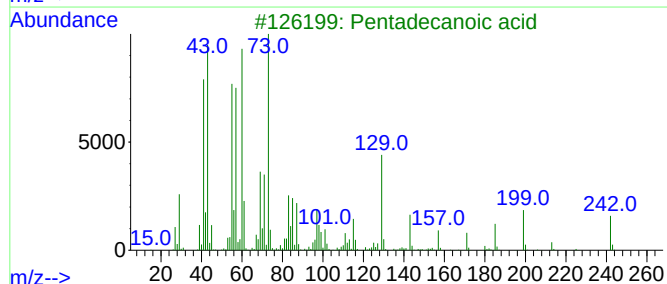
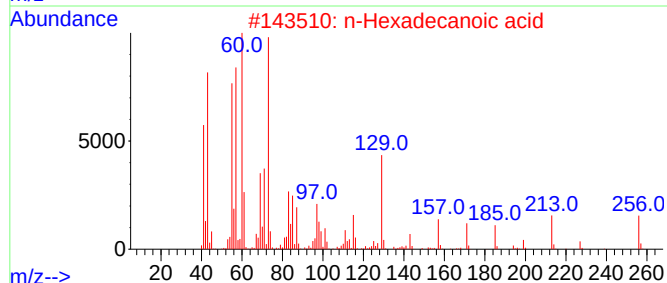
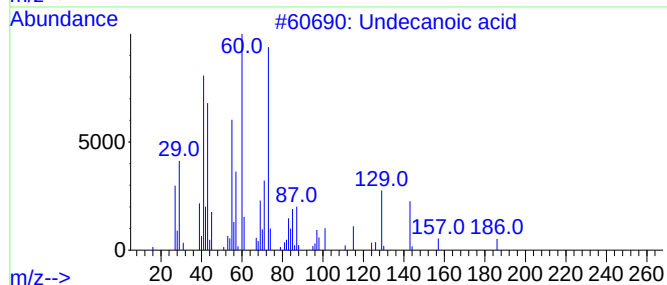
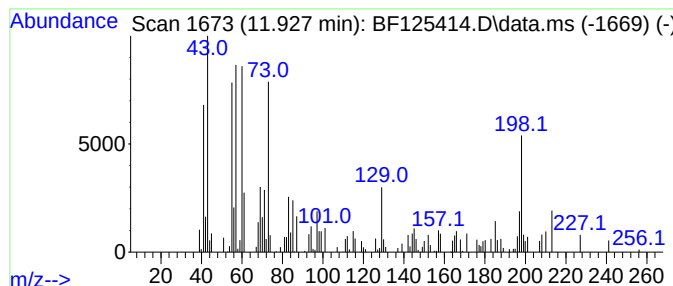
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Undecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.927	2.42 ng	127130	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecanoic acid	186	C11H22O2	000112-37-8	70
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	60
4			Lactose	342	C12H22O11	000063-42-3	38
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	38



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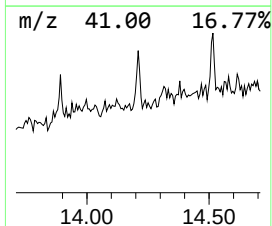
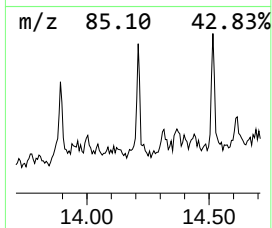
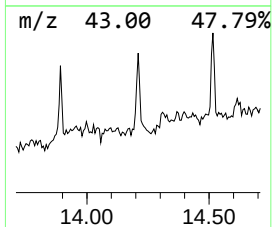
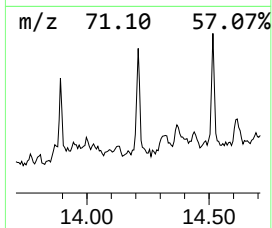
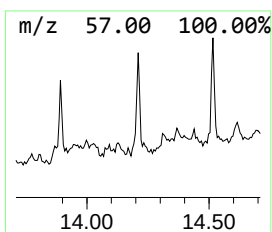
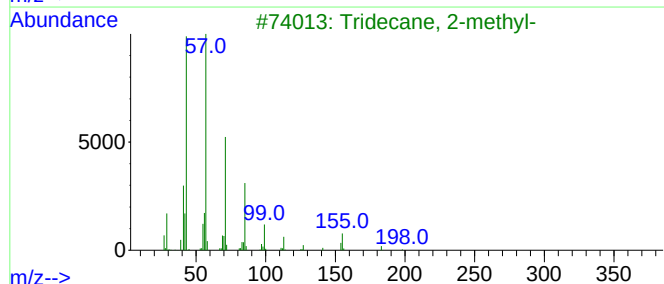
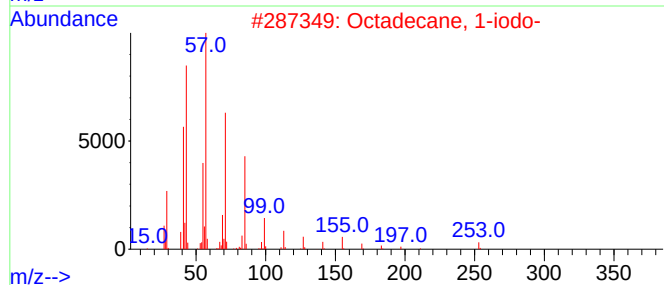
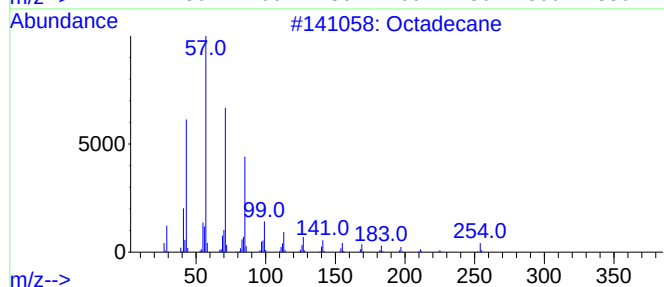
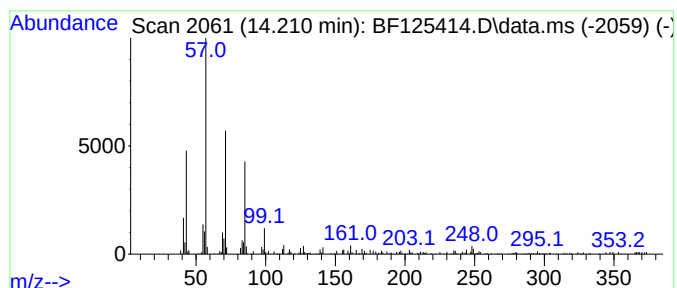
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Octadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.210	4.20 ng	196701	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	91
2			Octadecane, 1-iodo-	380	C18H37I	000629-93-6	80
3			Tridecane, 2-methyl-	198	C14H30	001560-96-9	80
4			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	80
5			Nonadecane	268	C19H40	000629-92-5	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090921\
Data File : BF125414.D
Acq On : 9 Sep 2021 15:56
Operator : JU/CG
Sample : M3680-03 5X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-SF-02-006-B

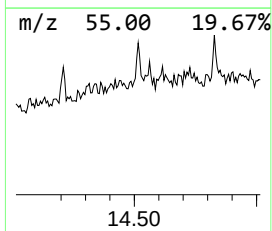
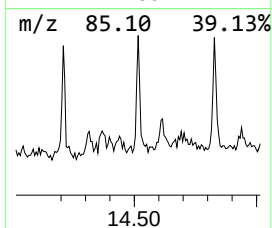
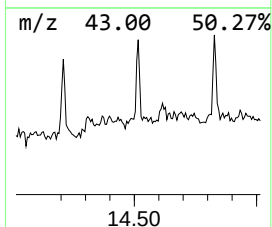
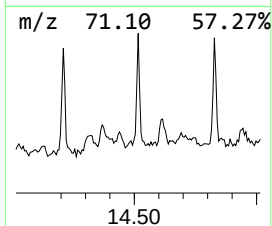
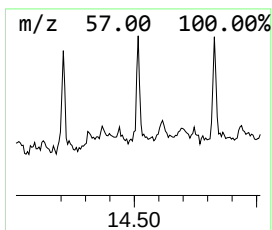
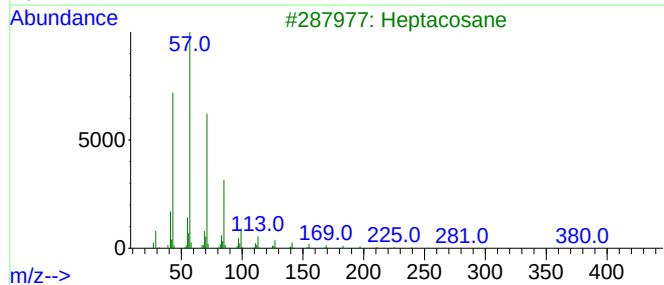
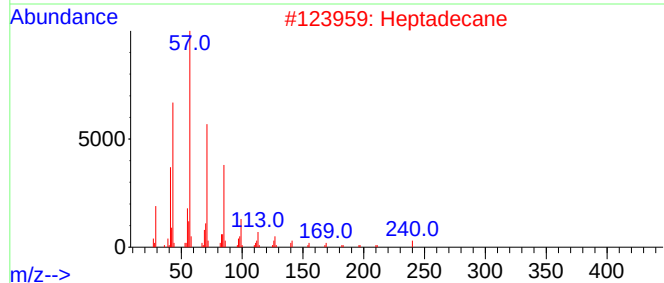
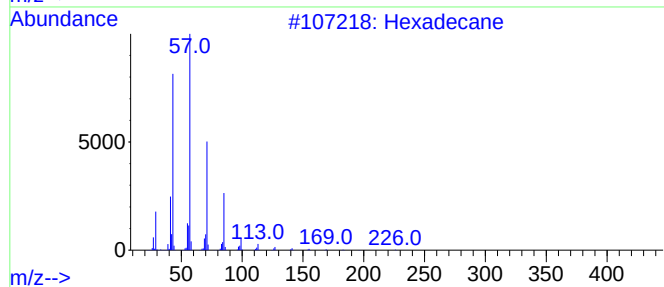
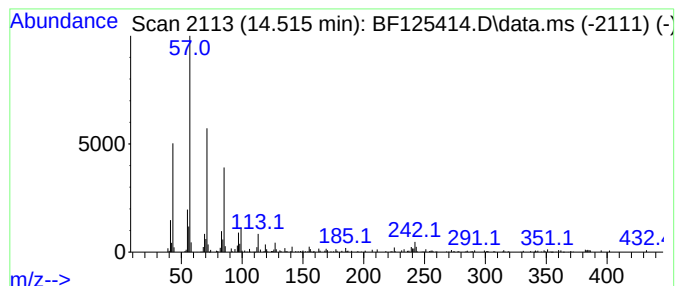
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.515	3.07 ng	143756	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	91
2			Heptadecane	240	C17H36	000629-78-7	91
3			Heptacosane	380	C27H56	000593-49-7	87
4			Hexacosane	366	C26H54	000630-01-3	80
5			Octadecane, 2-methyl-	268	C19H40	001560-88-9	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090921\
Data File : BF125414.D
Acq On : 9 Sep 2021 15:56
Operator : JU/CG
Sample : M3680-03 5X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-SF-02-006-B

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...	2.146	4.9	ng	237174	1	6.886	972109	20.0
Pentadecane, 2,...	10.833	3.3	ng	173413	4	11.416	1051970	20.0
Undecanoic acid	11.927	2.4	ng	127130	4	11.416	1051970	20.0
Octadecane	14.210	4.2	ng	196701	5	14.057	936348	20.0
Hexadecane	14.515	3.1	ng	143756	5	14.057	936348	20.0