

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100121\
 Data File : BF125748.D
 Acq On : 1 Oct 2021 12:37
 Operator : JU/CG
 Sample : PB139485BS
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB139485BS

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 1 % 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-BF092421.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125748.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.763	110	115	124	rVB	429068	619350	6.67%	0.201%
2	3.475	226	236	240	rBV	541647	1103017	11.87%	0.358%
3	3.516	240	243	268	rVB	676143	1476896	15.90%	0.479%
4	5.134	511	518	528	rVB	866293	1386653	14.92%	0.450%
5	5.522	578	584	587	rBV	5570395	6277108	67.56%	2.037%
6	6.439	736	740	743	rBV	2194242	1782038	19.18%	0.578%
7	6.522	747	754	758	rBV2	4842761	9291371	100.00%	3.015%
8	6.551	758	759	766	rVV	2280879	1791787	19.28%	0.581%
9	6.628	767	772	775	rVB	2348534	2038350	21.94%	0.661%
10	6.675	776	780	784	rBV	2921122	2737670	29.46%	0.888%
11	6.834	803	807	810	rBV	3698209	3087203	33.23%	1.002%
12	6.892	813	817	818	rBV	1698344	1791031	19.28%	0.581%
13	6.910	818	820	823	rVB	3807385	2836415	30.53%	0.920%
14	7.034	835	841	843	rBV	2713040	3122016	33.60%	1.013%
15	7.063	843	846	849	rVB	3321964	3062798	32.96%	0.994%
16	7.139	853	859	861	rBV	3135565	3498022	37.65%	1.135%
17	7.163	861	863	867	rVB	1840847	2100146	22.60%	0.682%
18	7.292	879	885	891	rBV3	5491305	7997182	86.07%	2.595%
19	7.404	900	904	907	rBV	2665786	2463754	26.52%	0.800%
20	7.457	907	913	914	rVV	3847388	4704249	50.63%	1.527%
21	7.475	914	916	919	rVB	2605072	1861497	20.03%	0.604%
22	7.563	928	931	935	rBV	429811	397839	4.28%	0.129%
23	7.710	950	956	964	rBV	2343301	3148030	33.88%	1.022%
24	7.786	964	969	971	rBV	2207367	1980944	21.32%	0.643%
25	7.822	971	975	978	rVV	3788971	3532150	38.02%	1.146%
26	7.922	981	992	994	rVV	2922236	3782417	40.71%	1.227%
27	7.951	994	997	1000	rVV	705609	925863	9.96%	0.300%
28	8.028	1004	1010	1013	rBV	3284741	2974920	32.02%	0.965%
29	8.116	1019	1025	1028	rVB	3311929	3437317	36.99%	1.115%
30	8.175	1029	1035	1036	rBV	2388319	2512700	27.04%	0.815%
31	8.198	1036	1039	1041	rVB	4573737	4205648	45.26%	1.365%
32	8.239	1041	1046	1049	rBV	2554726	2160175	23.25%	0.701%
33	8.310	1054	1058	1062	rVB	3049921	3038321	32.70%	0.986%
34	8.616	1105	1110	1113	rBV	936348	1175782	12.65%	0.382%
35	8.657	1113	1117	1123	rVV2	226297	611334	6.58%	0.198%
36	8.722	1123	1128	1131	rVB	3298742	2967113	31.93%	0.963%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100121\
 Data File : BF125748.D
 Acq On : 1 Oct 2021 12:37
 Operator : JU/CG
 Sample : PB139485BS
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB139485BS

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 1 % 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-BF092421.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	8.833	1140	1147	1151	rBV	1423987	1279114	13.77%	0.415%
38	8.886	1151	1156	1159	rVV	5463936	5048847	54.34%	1.638%
39	8.986	1167	1173	1176	rVV	5149051	4838117	52.07%	1.570%
40	9.045	1176	1183	1187	rVB3	5111896	7222268	77.73%	2.344%
41	9.163	1196	1203	1205	rBV	3391562	3308124	35.60%	1.074%
42	9.180	1205	1206	1207	rVV	1264531	846407	9.11%	0.275%
43	9.204	1207	1210	1213	rVV	2984907	2956498	31.82%	0.959%
44	9.251	1213	1218	1221	rVB	7832529	7899168	85.02%	2.563%
45	9.351	1228	1235	1237	rBV	5873049	5425620	58.39%	1.761%
46	9.375	1237	1239	1242	rVB	4736389	3943785	42.45%	1.280%
47	9.469	1247	1255	1258	rBV	2520679	2383038	25.65%	0.773%
48	9.604	1274	1278	1280	rVV	1848028	1575313	16.95%	0.511%
49	9.651	1280	1286	1288	rVV	3836092	3536067	38.06%	1.148%
50	9.680	1288	1291	1293	rVV	1703088	1781086	19.17%	0.578%
51	9.710	1293	1296	1299	rVB	2883257	2273224	24.47%	0.738%
52	9.769	1299	1306	1307	rBV	1563777	1457301	15.68%	0.473%
53	9.792	1307	1310	1313	rVB	5064456	4407407	47.44%	1.430%
54	9.880	1321	1325	1328	rVB	1814084	1720075	18.51%	0.558%
55	9.927	1328	1333	1336	rBV	2720609	2529345	27.22%	0.821%
56	9.963	1336	1339	1341	rVV	5722291	5473507	58.91%	1.776%
57	9.986	1341	1343	1346	rVV	2464962	1746225	18.79%	0.567%
58	10.039	1346	1352	1355	rVV	2810274	2937560	31.62%	0.953%
59	10.075	1355	1358	1361	rVV	986141	915193	9.85%	0.297%
60	10.116	1361	1365	1366	rVV	2626350	2403819	25.87%	0.780%
61	10.133	1366	1368	1372	rVB	4613861	4067161	43.77%	1.320%
62	10.204	1376	1380	1384	rBV	2894008	2724539	29.32%	0.884%
63	10.251	1384	1388	1391	rVB	3318331	2742873	29.52%	0.890%
64	10.351	1398	1405	1408	rBV	3951788	3649228	39.28%	1.184%
65	10.474	1420	1426	1429	rBV2	5828031	8974754	96.59%	2.913%
66	10.522	1431	1434	1437	rVV	1708552	1328255	14.30%	0.431%
67	10.586	1438	1445	1448	rVV	5098304	4701952	50.61%	1.526%
68	10.627	1448	1452	1455	rVB	4072392	3481736	37.47%	1.130%
69	10.722	1461	1468	1471	rBV	4572315	4693076	50.51%	1.523%
70	10.957	1504	1508	1511	rBV	3634704	2924887	31.48%	0.949%
71	11.027	1514	1520	1523	rBV	3603574	3205085	34.50%	1.040%
72	11.110	1527	1534	1537	rBV	3164203	2953742	31.79%	0.959%
73	11.216	1548	1552	1563	rBV	4345178	4225375	45.48%	1.371%
74	11.416	1581	1586	1587	rBV	2195736	2237525	24.08%	0.726%
75	11.439	1587	1590	1593	rVV	5476731	4799582	51.66%	1.558%
76	11.492	1593	1599	1602	rVB	5407720	4787981	51.53%	1.554%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100121\
 Data File : BF125748.D
 Acq On : 1 Oct 2021 12:37
 Operator : JU/CG
 Sample : PB139485BS
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB139485BS

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 1 % 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

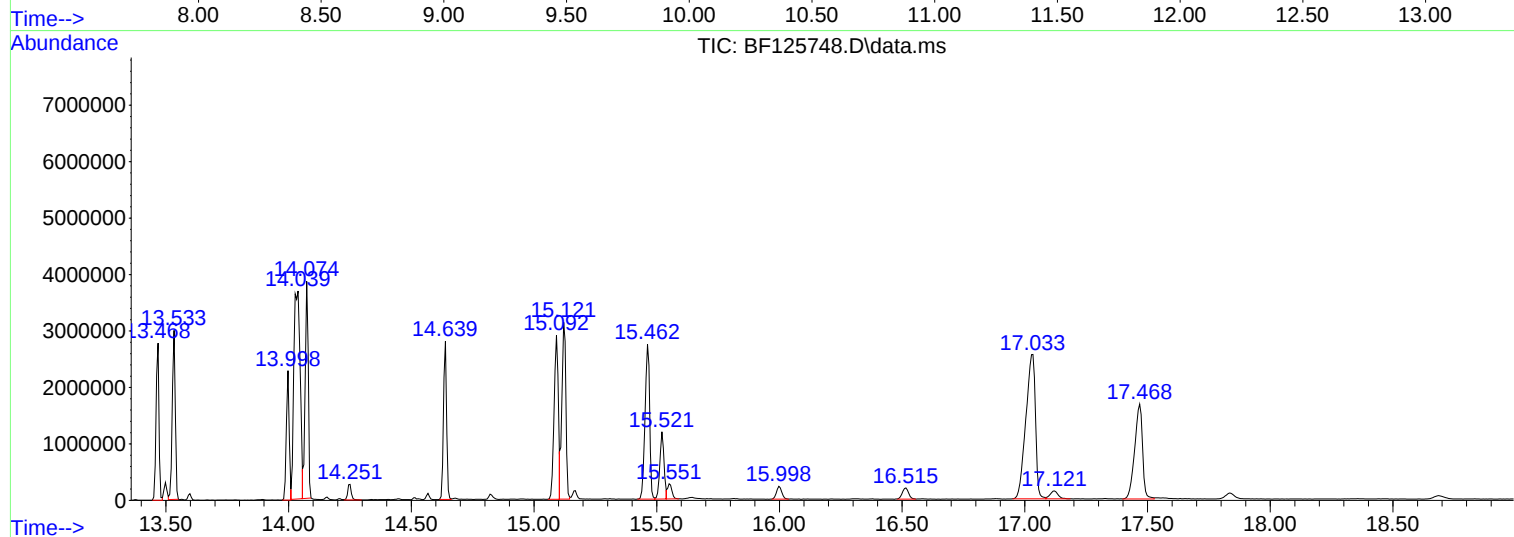
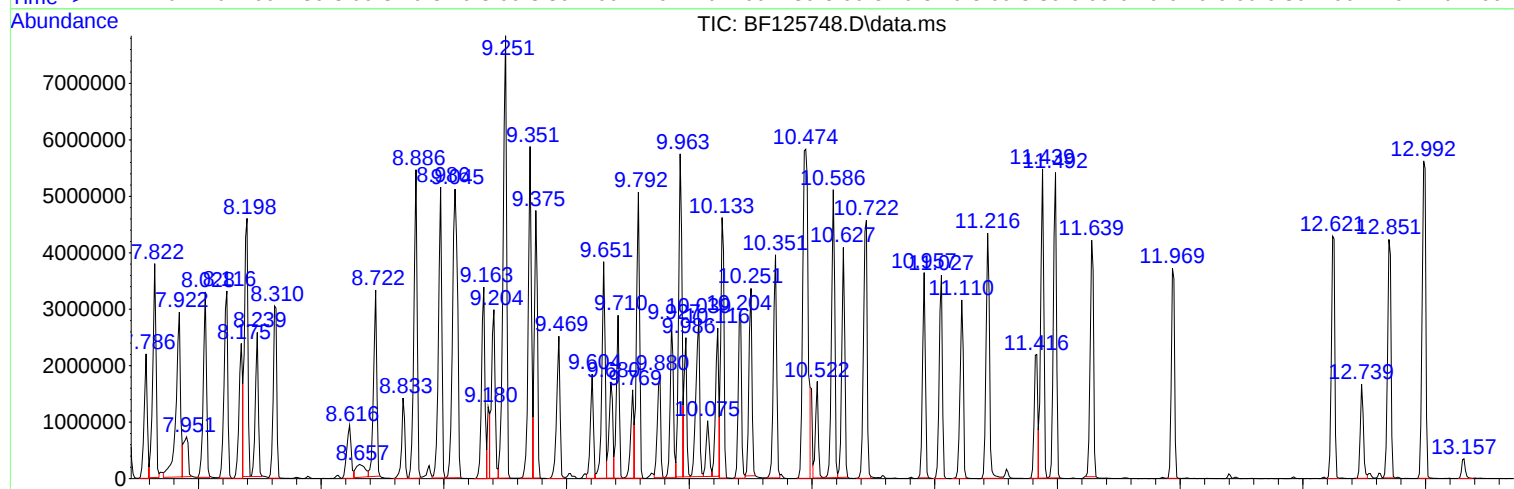
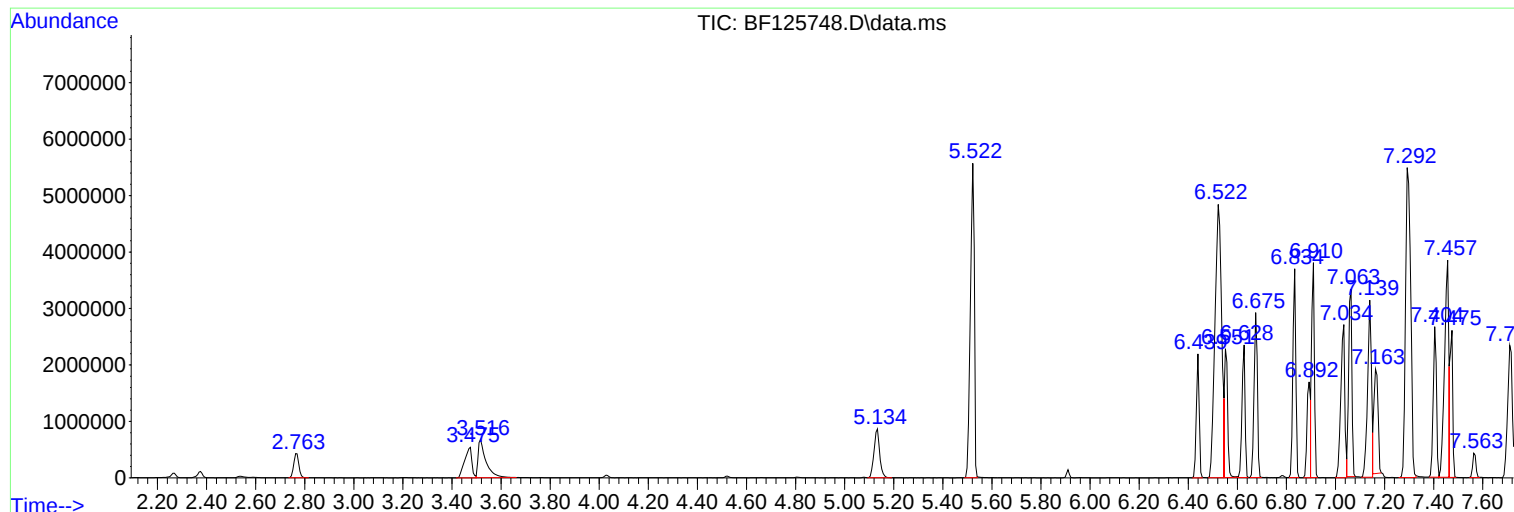
Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

77	11.639	1620	1624	1627	rVB	4192607	3997357	43.02%	1.297%
78	11.969	1676	1680	1684	rBV	3721772	3404144	36.64%	1.105%
79	12.621	1787	1791	1795	rBV	4291458	4144238	44.60%	1.345%
80	12.739	1807	1811	1815	rBV	1668544	1466501	15.78%	0.476%
81	12.851	1826	1830	1834	rVB	4224381	4118996	44.33%	1.337%
82	12.992	1850	1854	1858	rBV	5624975	5826865	62.71%	1.891%
83	13.157	1878	1882	1888	rBV	347855	356553	3.84%	0.116%
84	13.468	1931	1935	1938	rBV	2782942	2295838	24.71%	0.745%
85	13.533	1942	1946	1949	rVB	2994117	2554218	27.49%	0.829%
86	13.998	2021	2025	2027	rBV	2292694	1877545	20.21%	0.609%
87	14.039	2027	2032	2035	rVV3	3686158	6664546	71.73%	2.163%
88	14.074	2035	2038	2041	rVB	3841107	3369352	36.26%	1.093%
89	14.251	2064	2068	2076	rVB	274644	281597	3.03%	0.091%
90	14.639	2130	2134	2138	rBV	2804852	2464419	26.52%	0.800%
91	15.092	2205	2211	2213	rBV	2900914	3517260	37.86%	1.141%
92	15.121	2213	2216	2220	rVV	3132765	3463986	37.28%	1.124%
93	15.462	2267	2274	2279	rBV	2742466	3600175	38.75%	1.168%
94	15.521	2279	2284	2287	rVV	1189289	1402901	15.10%	0.455%
95	15.551	2287	2289	2296	rVB	267777	323866	3.49%	0.105%
96	15.998	2360	2365	2372	rVB	226139	337316	3.63%	0.109%
97	16.515	2447	2453	2460	rVB	196859	348364	3.75%	0.113%
98	17.033	2527	2541	2550	rBV3	2555830	6989891	75.23%	2.268%
99	17.121	2550	2556	2567	rVB	140297	316157	3.40%	0.103%
100	17.468	2603	2615	2625	rBV	1679633	3738107	40.23%	1.213%

Sum of corrected areas: 308144157

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100121\
Data File : BF125748.D
Acq On : 1 Oct 2021 12:37
Operator : JU/CG
Sample : PB139485BS
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB139485BS

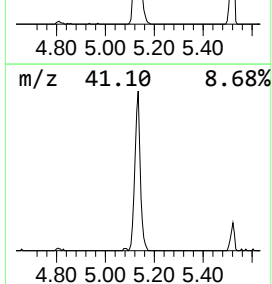
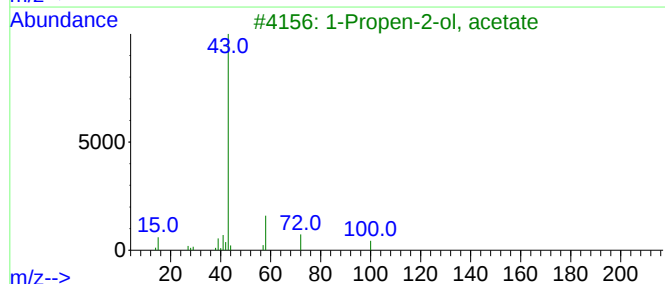
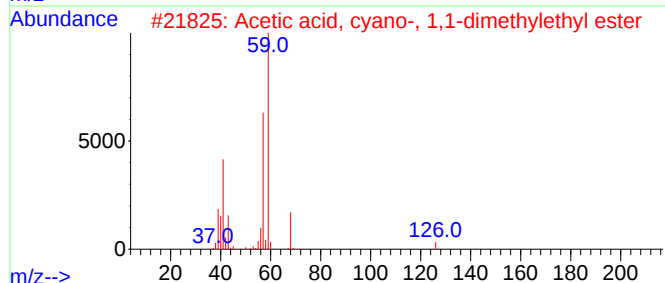
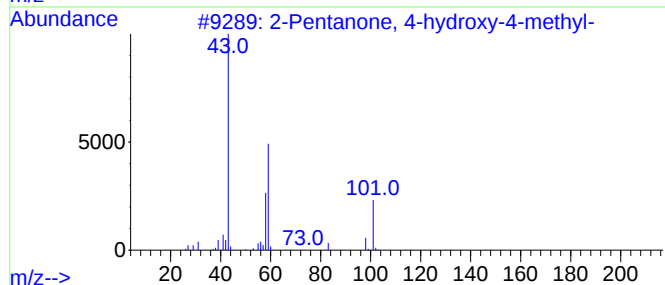
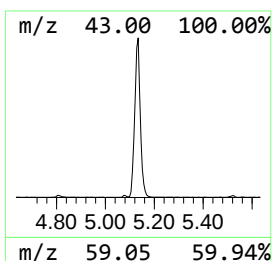
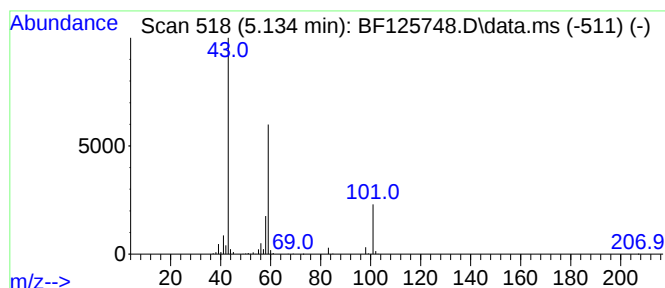
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.134	15.48 ng	1386650	1,4-Dichlorobenzene-d4	6.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100121\
Data File : BF125748.D
Acq On : 1 Oct 2021 12:37
Operator : JU/CG
Sample : PB139485BS
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB139485BS

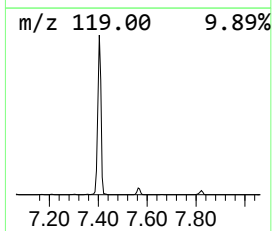
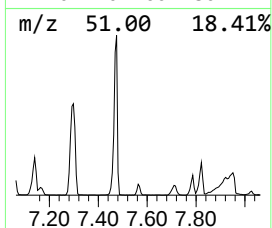
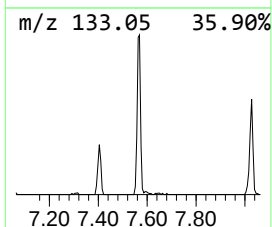
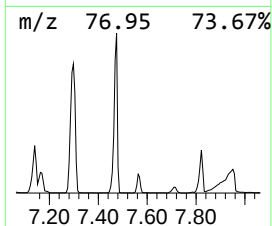
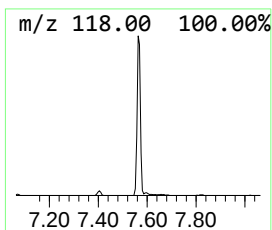
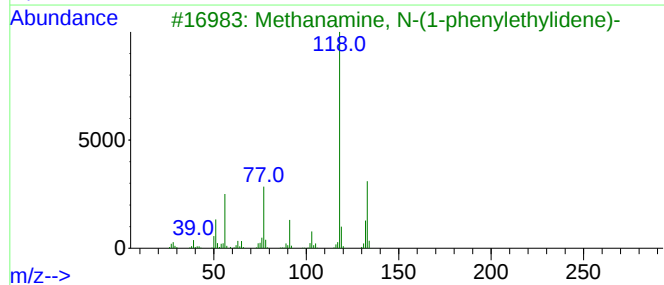
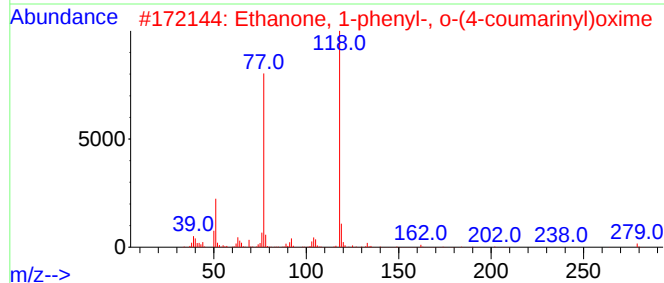
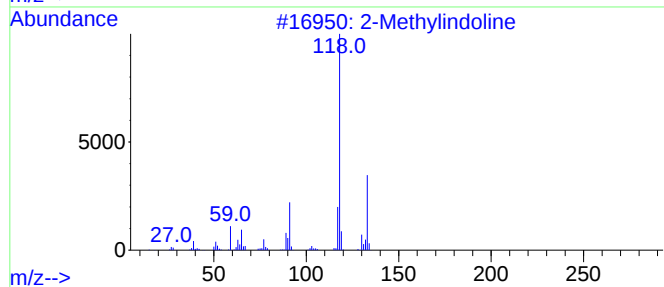
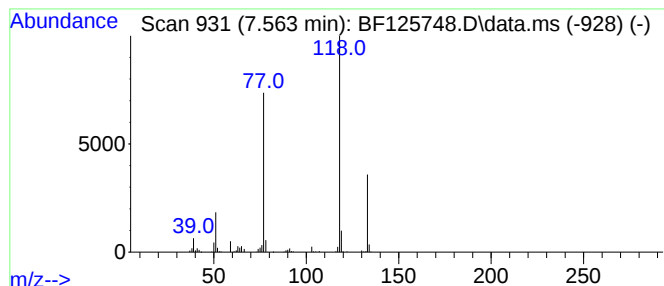
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Methylindoline Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.563	3.17 ng	397839	Naphthalene-d8	8.175

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methylindoline	133	C9H11N	006872-06-6	43
2			Ethanone, 1-phenyl-, o-(4-coumar...	279	C17H13NO3	034605-11-3	35
3			Methanamine, N-(1-phenylethylide...	133	C9H11N	006907-71-7	28
4			1H-Benzimidazole	118	C7H6N2	000051-17-2	27
5			Benzenecarboximidoyl bromide, N-...	197	C8H8BrN	041182-85-8	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100121\
Data File : BF125748.D
Acq On : 1 Oct 2021 12:37
Operator : JU/CG
Sample : PB139485BS
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB139485BS

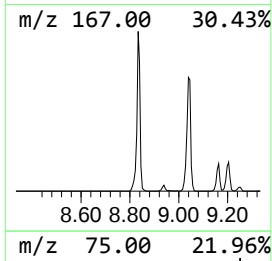
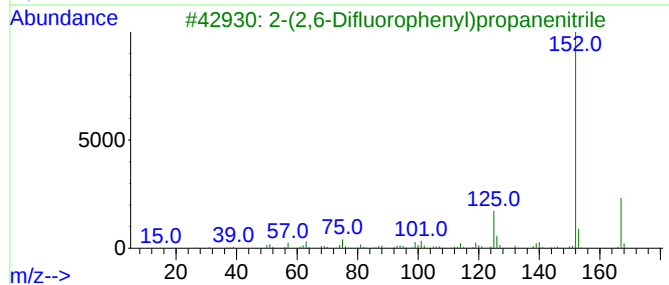
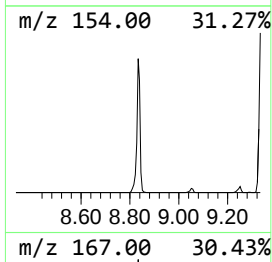
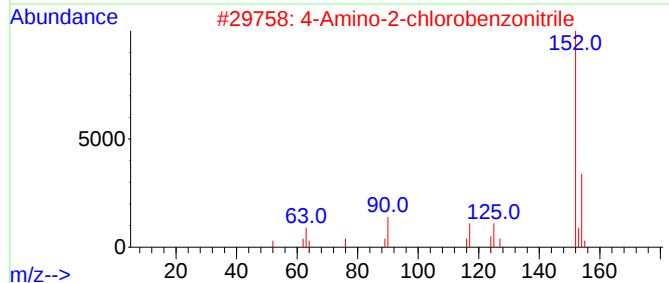
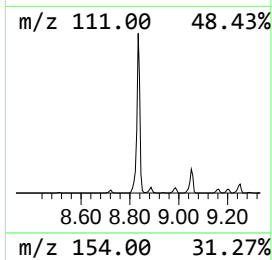
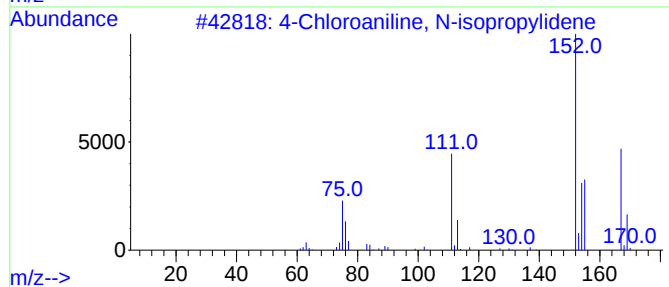
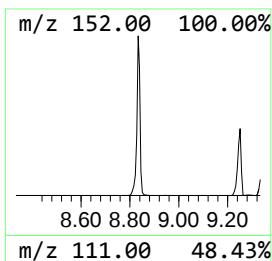
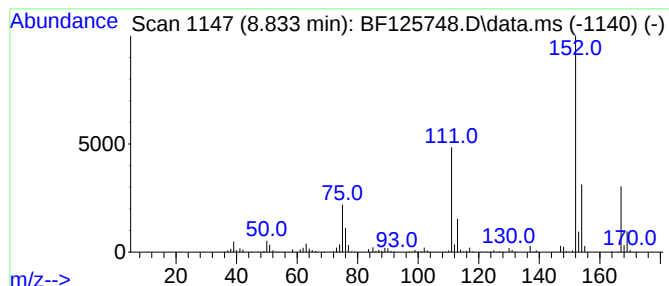
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 4-Chloroaniline, N-isopropy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.833	10.18 ng	1279110	Naphthalene-d8	8.175

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		4-Chloroaniline, N-isopropylidene	167	C9H10ClN	040938-43-0	94
2		4-Amino-2-chlorobenzonitrile	152	C7H5ClN2	020925-27-3	38
3		2-(2,6-Difluorophenyl)propanenit...	167	C9H7F2N	149680-18-2	38
4		Benzonitrile, 2-amino-5-chloro-	152	C7H5ClN2	005922-60-1	38
5		5-Aminopyrimidine, N-trimethylsi...	167	C7H13N3Si	1000493-88-4	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100121\
Data File : BF125748.D
Acq On : 1 Oct 2021 12:37
Operator : JU/CG
Sample : PB139485BS
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB139485BS

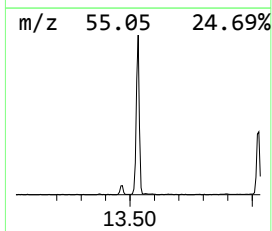
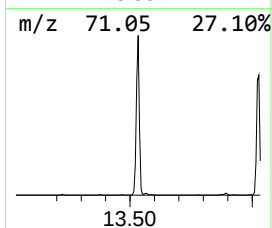
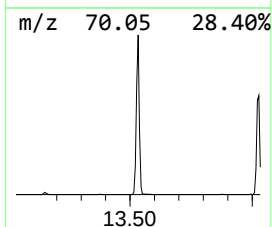
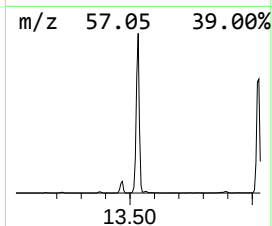
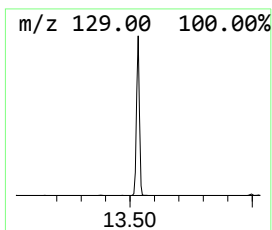
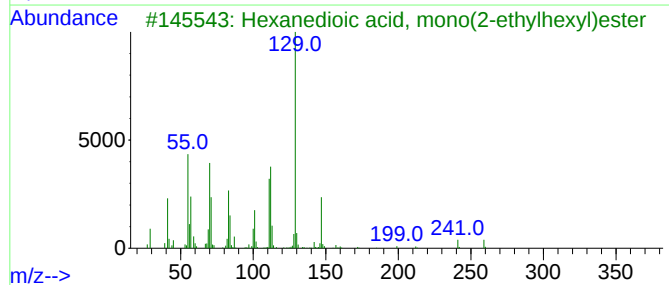
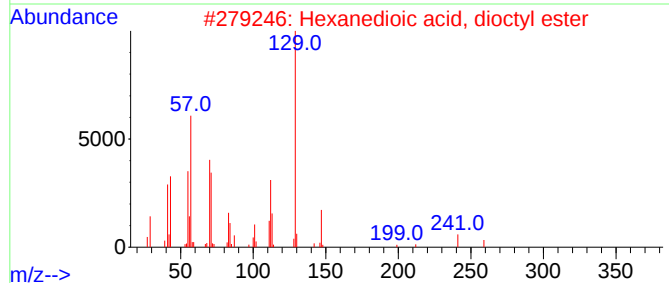
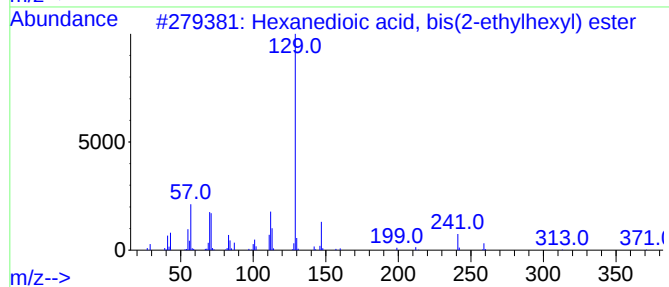
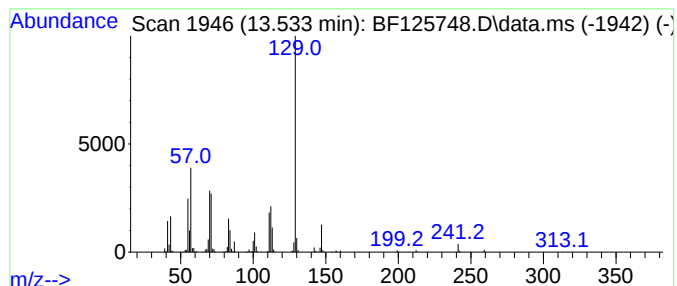
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Hexanedioic acid, bis(2-eth... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.533	7.67 ng	2554220	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	91
2			Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	76
3			Hexanedioic acid, mono(2-ethylhe...	258	C14H26O4	004337-65-9	68
4			Adipic acid, 2-ethylhexyl isobut...	314	C18H34O4	1010324-48-0	64
5			Diisooctyl adipate	370	C22H42O4	001330-86-5	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100121\
Data File : BF125748.D
Acq On : 1 Oct 2021 12:37
Operator : JU/CG
Sample : PB139485BS
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB139485BS

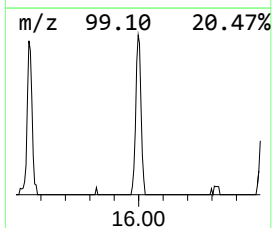
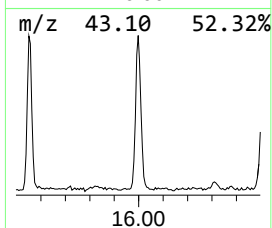
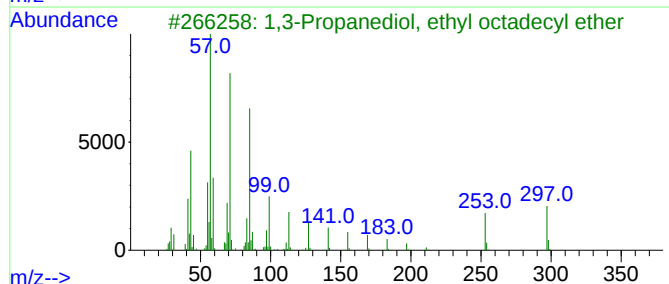
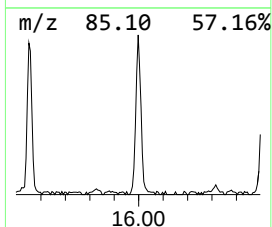
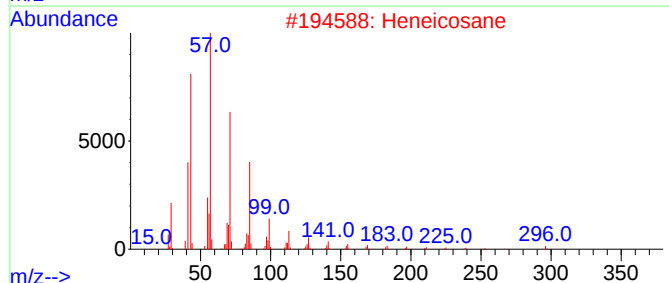
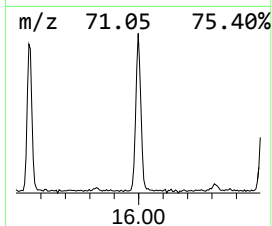
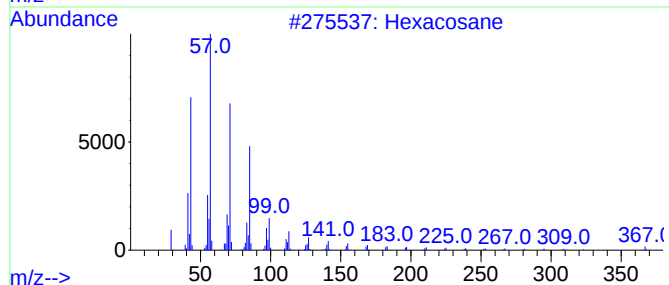
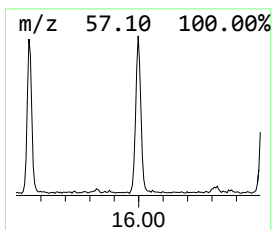
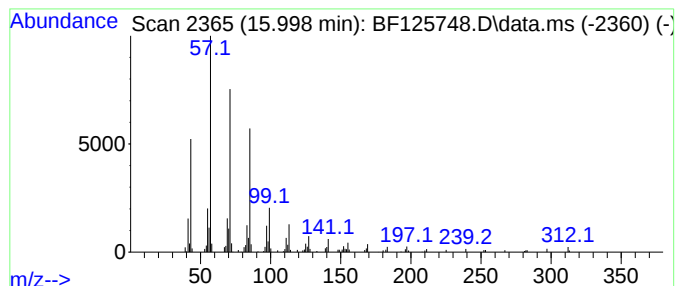
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.998	4.81 ng	337316	Perylene-d12	15.521

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	91
2			Heneicosane	296	C21H44	000629-94-7	91
3			1,3-Propanediol, ethyl octadecyl...	356	C23H48O2	1000406-35-4	91
4			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
5			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100121\
Data File : BF125748.D
Acq On : 1 Oct 2021 12:37
Operator : JU/CG
Sample : PB139485BS
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB139485BS

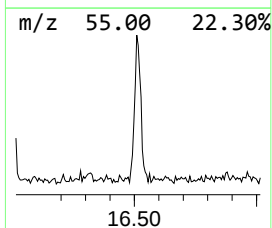
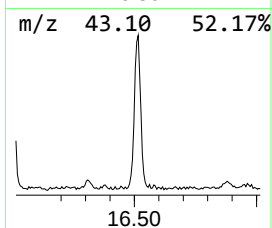
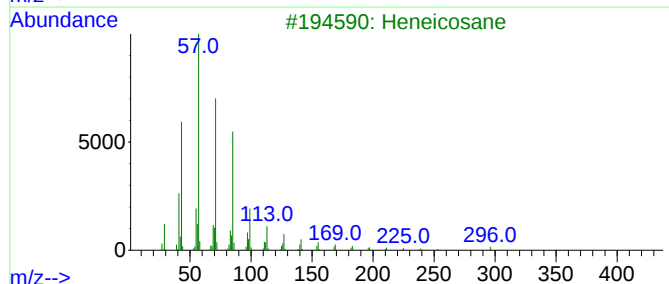
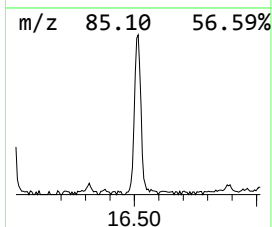
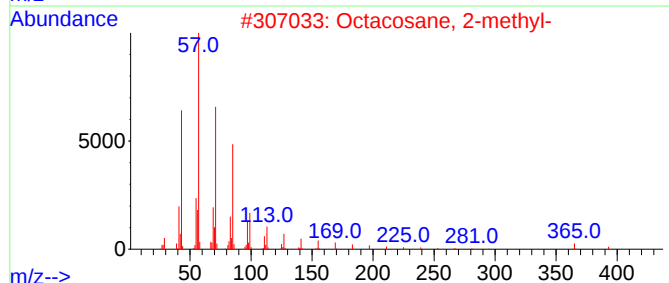
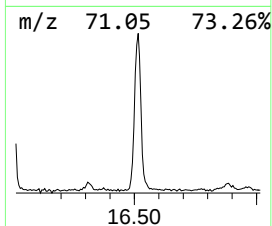
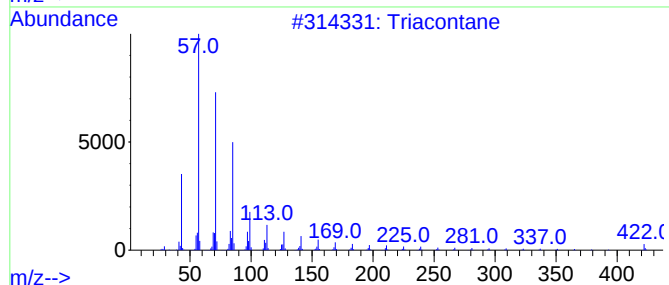
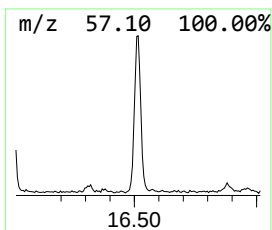
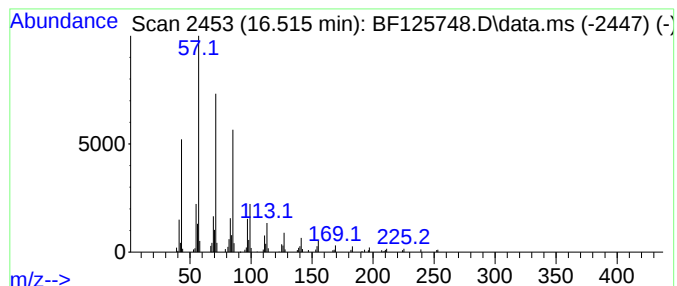
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Triacontane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.515	4.97 ng	348364	Perylene-d12	15.521

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triacontane	422	C30H62	000638-68-6	91
2			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
3			Heneicosane	296	C21H44	000629-94-7	91
4			Hexacosane	366	C26H54	000630-01-3	91
5			Pentacosane	352	C25H52	000629-99-2	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100121\
Data File : BF125748.D
Acq On : 1 Oct 2021 12:37
Operator : JU/CG
Sample : PB139485BS
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB139485BS

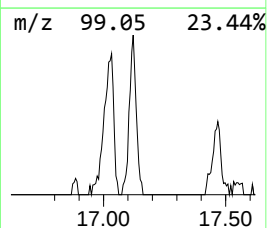
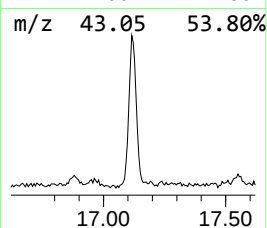
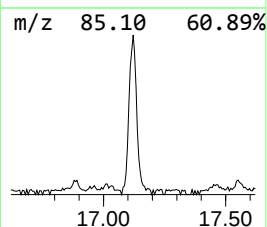
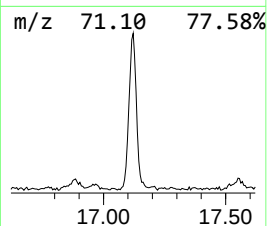
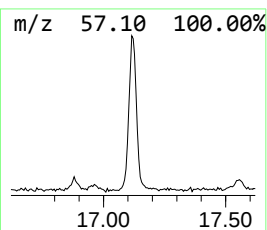
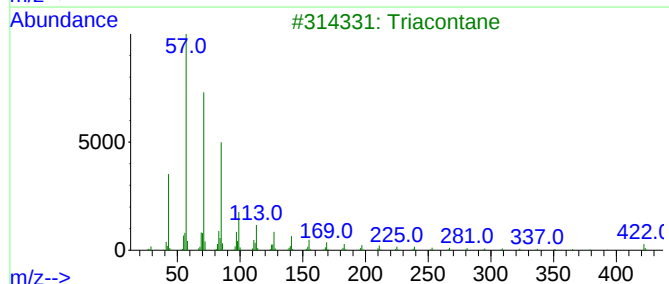
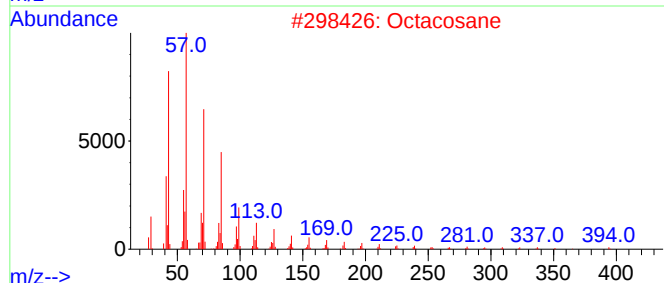
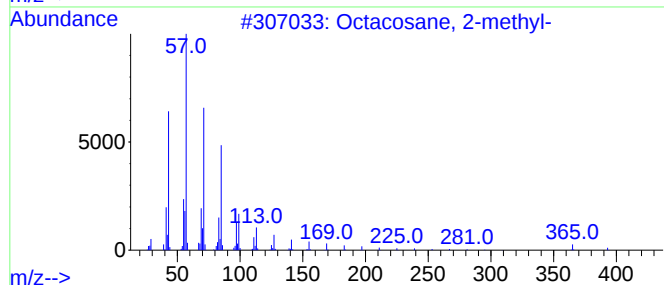
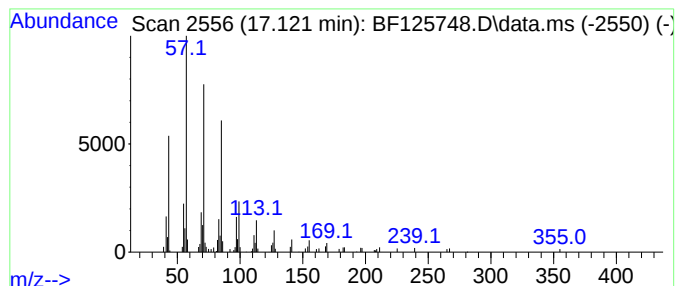
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octacosane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.121	4.51 ng	316157	Perylene-d12	15.521

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
2			Octacosane	394	C28H58	000630-02-4	91
3			Triacontane	422	C30H62	000638-68-6	91
4			4-Methylheneicosane	310	C22H46	025117-29-7	91
5			Tetracosane	338	C24H50	000646-31-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100121\
Data File : BF125748.D
Acq On : 1 Oct 2021 12:37
Operator : JU/CG
Sample : PB139485BS
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB139485BS

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.134	15.5	ng	1386650	1	6.892	1791030	20.0
2-Methylindoline	7.563	3.2	ng	397839	2	8.175	2512700	20.0
4-Chloroaniline...	8.833	10.2	ng	1279110	2	8.175	2512700	20.0
Hexanedioic aci...	13.533	7.7	ng	2554220	5	14.051	6664550	20.0
Hexacosane	15.998	4.8	ng	337316	6	15.521	1402900	20.0
Triacotane	16.515	5.0	ng	348364	6	15.521	1402900	20.0
Octacosane, 2-m...	17.121	4.5	ng	316157	6	15.521	1402900	20.0