

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032125\
 Data File : BF142033.D
 Acq On : 21 Mar 2025 16:51
 Operator : RC/JU
 Sample : Q1619-11
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-4

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-BF031025.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF142033.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.163	4	12	23	rVV	879217	1408427	38.82%	5.074%
2	2.258	23	28	44	rVB	25628	53664	1.48%	0.193%
3	4.481	400	406	413	rBV	171952	260516	7.18%	0.938%
4	5.093	501	510	525	rBV	108561	182498	5.03%	0.657%
5	5.493	572	578	583	rBV	2018109	2665974	73.48%	9.604%
6	6.493	742	748	766	rBV	1909754	2729480	75.23%	9.832%
7	6.875	808	813	820	rBV	660622	832513	22.95%	2.999%
8	7.434	897	908	917	rBV	1342084	1795297	49.48%	6.467%
9	7.687	947	951	960	rVB	48014	64347	1.77%	0.232%
10	8.151	1025	1030	1039	rBV2	820634	1472553	40.59%	5.305%
11	8.369	1062	1067	1073	rVB2	30619	46218	1.27%	0.166%
12	8.869	1147	1152	1157	rBV	119784	155469	4.29%	0.560%
13	8.922	1157	1161	1164	rVV	26607	37236	1.03%	0.134%
14	8.963	1164	1168	1175	rVB	76379	98810	2.72%	0.356%
15	9.228	1207	1213	1222	rBV	2891323	3628166	100.00%	13.070%
16	9.310	1223	1227	1235	rVB4	18382	42808	1.18%	0.154%
17	9.563	1266	1270	1274	rBV	32427	52268	1.44%	0.188%
18	9.681	1287	1290	1300	rVB4	17430	37564	1.04%	0.135%
19	9.910	1321	1329	1332	rBV	963521	1307488	36.04%	4.710%
20	9.939	1332	1334	1339	rVB	569088	631686	17.41%	2.276%
21	10.110	1359	1363	1368	rBV	340352	444530	12.25%	1.601%
22	10.457	1417	1422	1427	rBV	307584	398817	10.99%	1.437%
23	10.522	1427	1433	1434	rBV	25281	36479	1.01%	0.131%
24	10.622	1445	1450	1456	rVB	240933	327868	9.04%	1.181%
25	10.692	1457	1462	1478	rVV	1509876	2058227	56.73%	7.414%
26	10.822	1479	1484	1491	rVB2	32735	56131	1.55%	0.202%
27	11.292	1560	1564	1569	rVB2	53472	76836	2.12%	0.277%
28	11.392	1576	1581	1584	rBV	851398	1232311	33.97%	4.439%
29	11.622	1616	1620	1628	rBV	48135	80761	2.23%	0.291%
30	11.916	1665	1670	1676	rBV3	55234	100701	2.78%	0.363%
31	12.010	1682	1686	1693	rVB	61173	98534	2.72%	0.355%
32	12.604	1783	1787	1791	rBV	114055	152757	4.21%	0.550%
33	12.645	1791	1794	1799	rVB	63333	80200	2.21%	0.289%
34	12.704	1800	1804	1811	rBV2	41096	76156	2.10%	0.274%
35	12.833	1822	1826	1834	rVB	109352	155293	4.28%	0.559%
36	12.980	1845	1851	1859	rBV	2180803	2892599	79.73%	10.420%

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Instrument :
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ClientSampleId :
TP-4

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-BF031025.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.875	1998	2003	2013	rBV2	98043	209281	5.77%	0.754%
38	14.033	2024	2030	2041	rVB	555042	836290	23.05%	3.013%
39	14.880	2170	2174	2179	rVB	81662	114032	3.14%	0.411%
40	15.504	2274	2280	2292	rVB	512497	829035	22.85%	2.986%

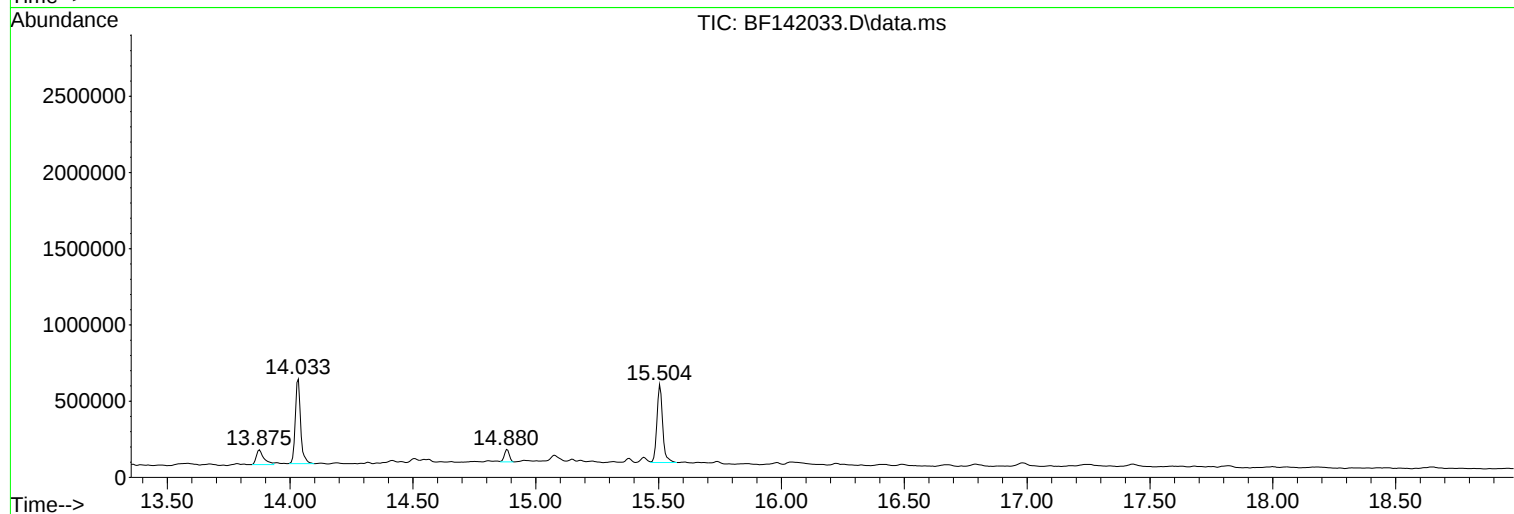
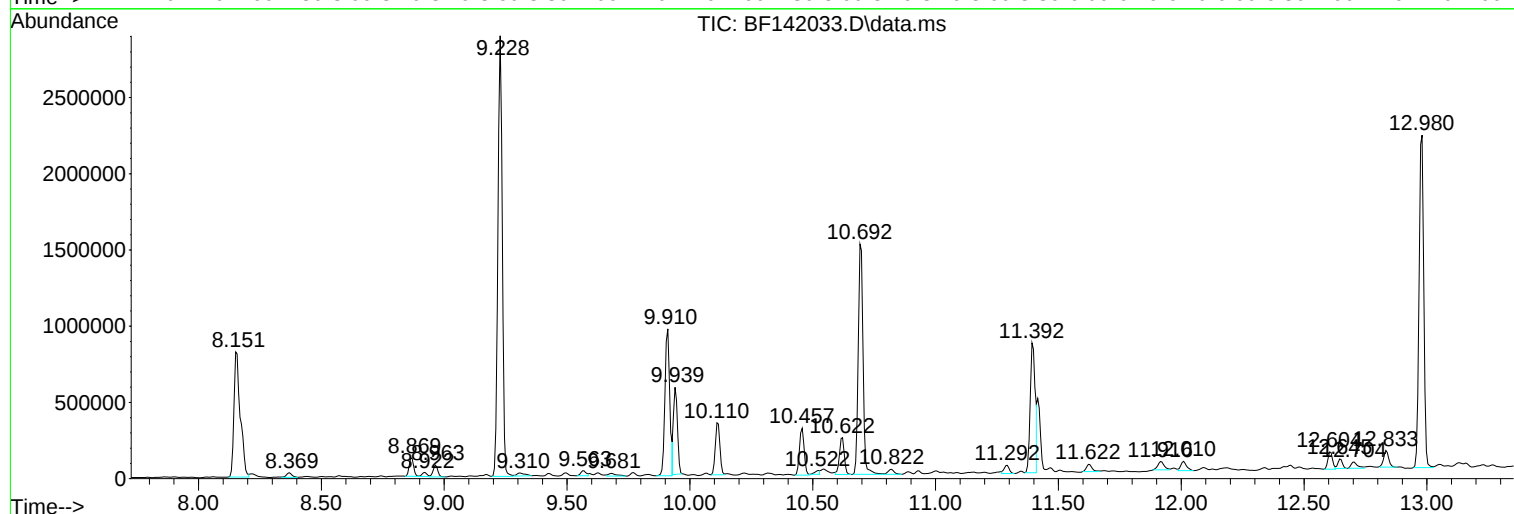
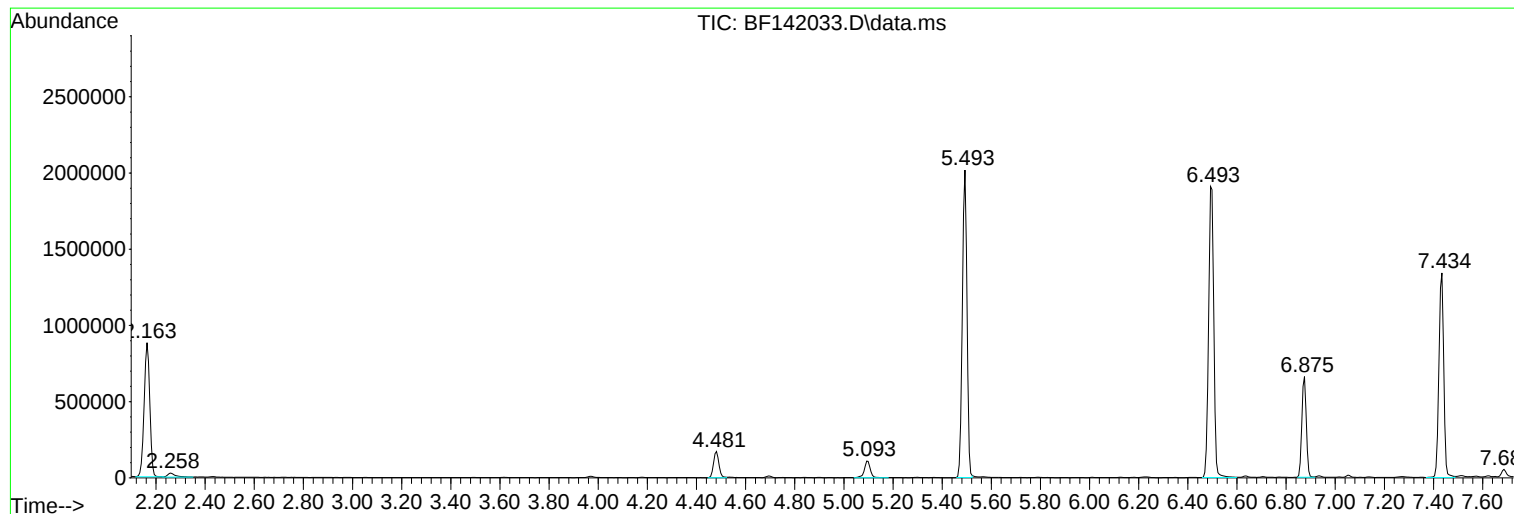
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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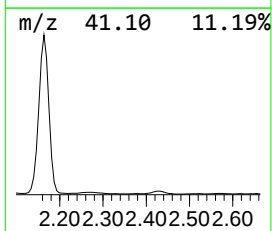
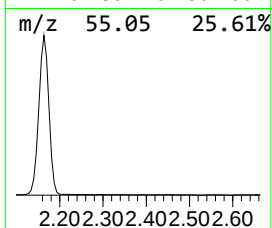
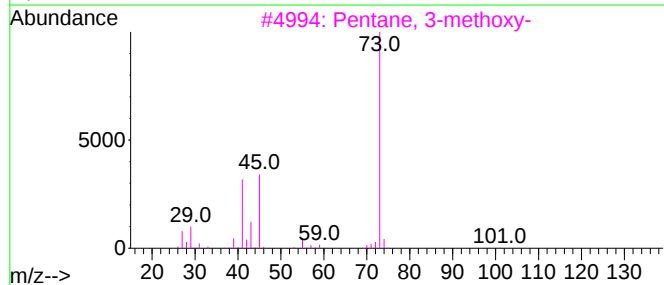
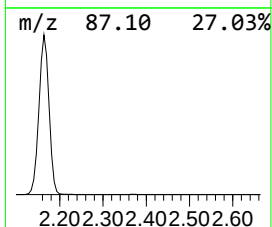
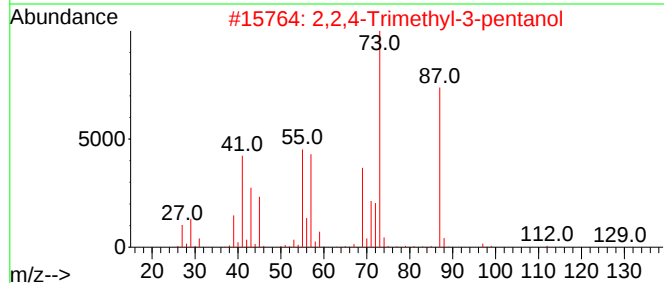
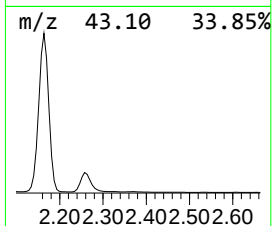
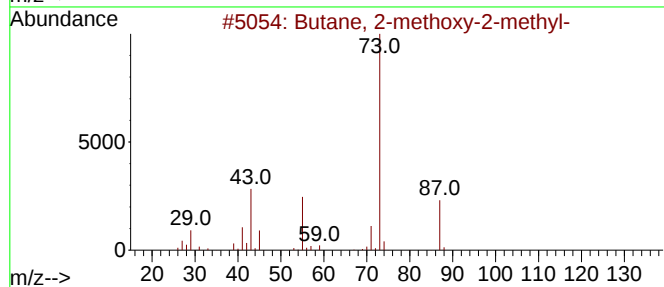
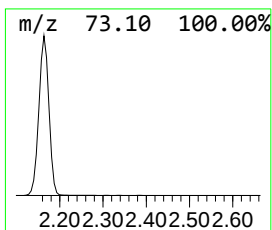
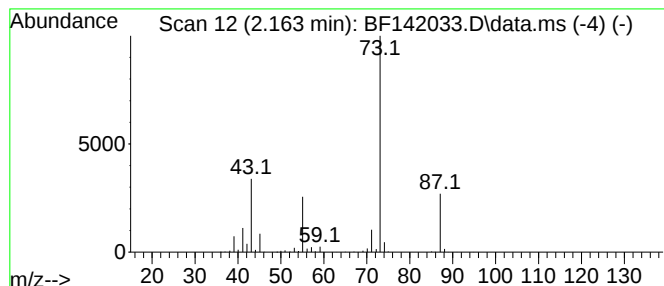
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.163	33.84 ng	1408430	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4			N-Ethylformamide	73	C3H7NO	000627-45-2	9
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9



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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4

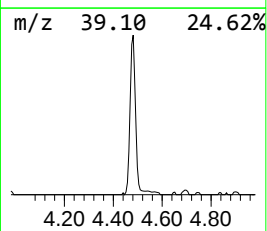
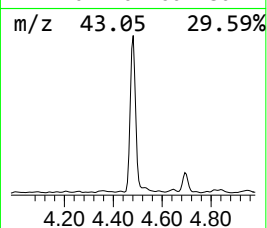
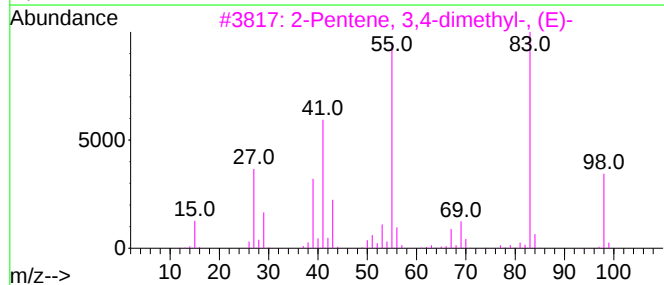
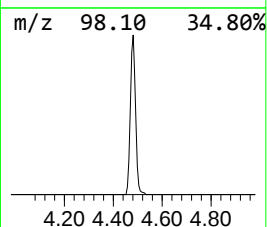
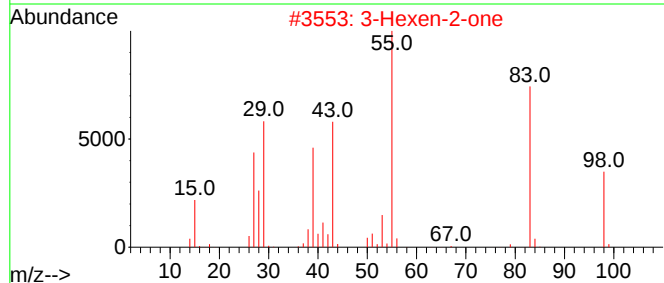
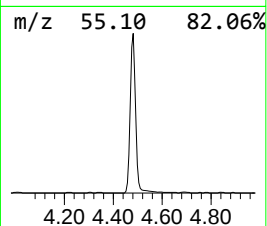
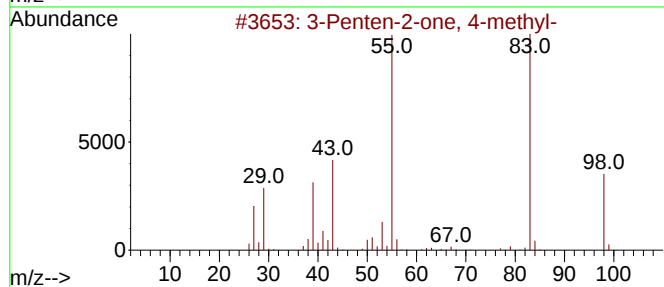
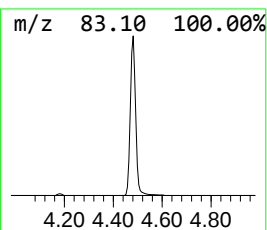
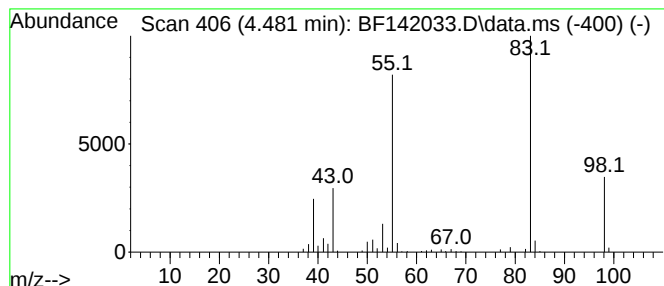
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.481	6.26 ng	260516	1,4-Dichlorobenzene-d4	6.875

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2		3-Hexen-2-one	98	C6H10O	000763-93-9	91
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80



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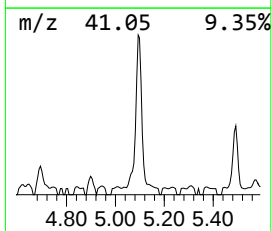
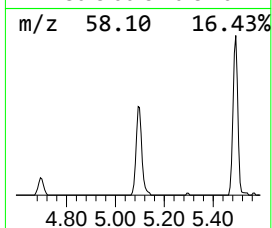
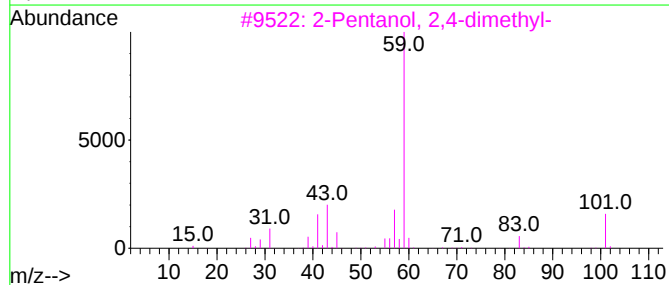
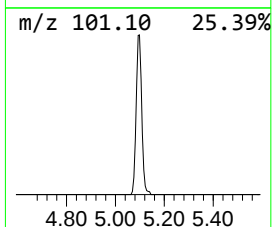
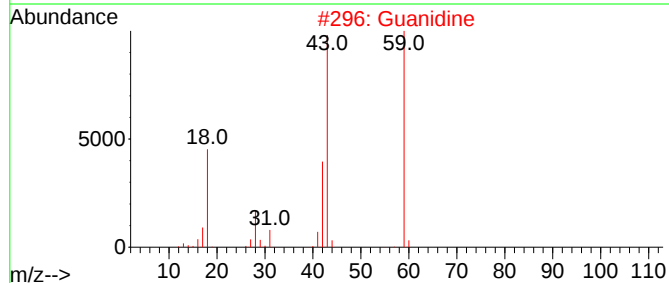
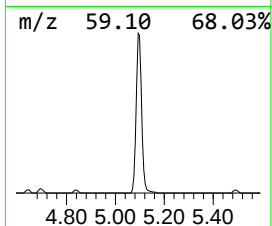
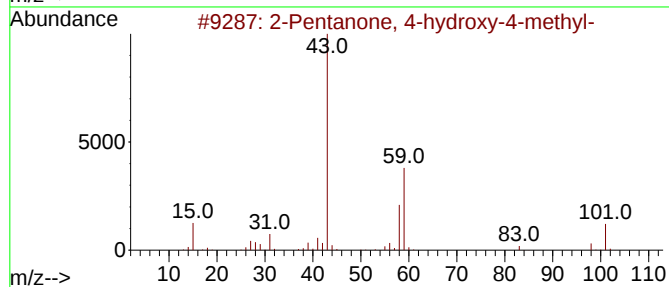
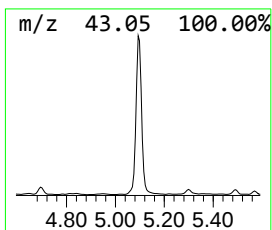
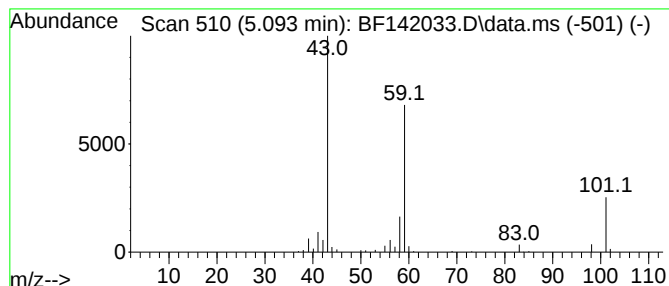
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.093	4.38 ng	182498	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Guanidine	59	CH5N3	000113-00-8	43
3			2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	42
4			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	23
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17



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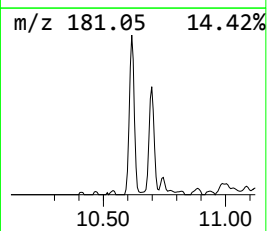
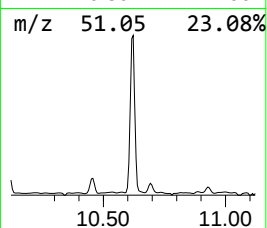
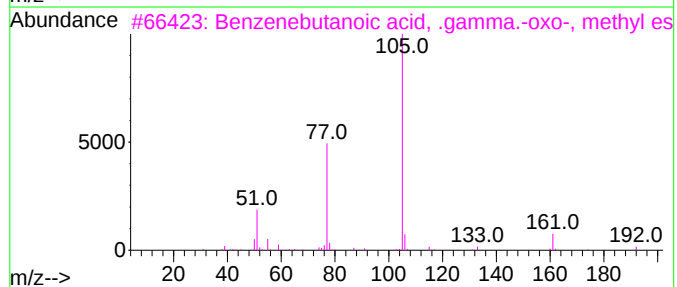
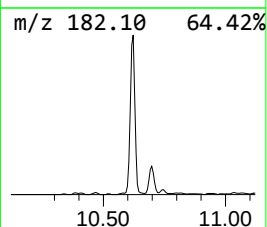
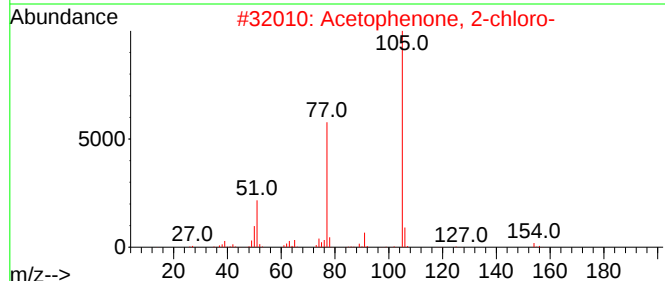
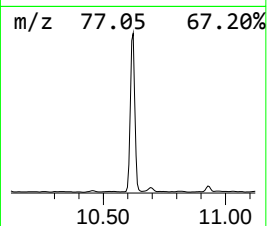
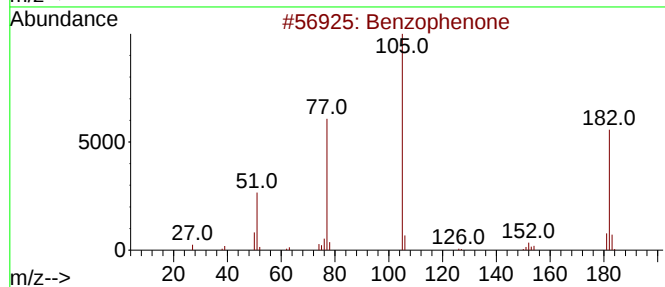
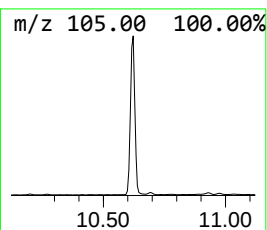
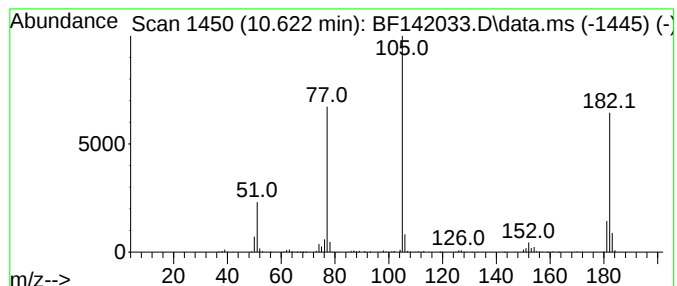
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.622	5.02 ng	327868	Acenaphthene-d10	9.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3			Benzenebutanoic acid, .gamma.-ox...	192	C11H12O3	025333-24-8	47
4			Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	47
5			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47



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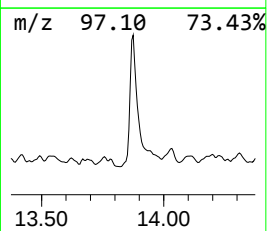
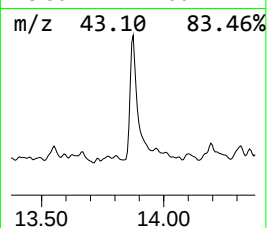
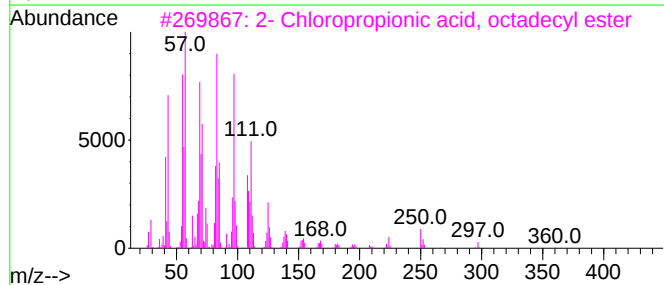
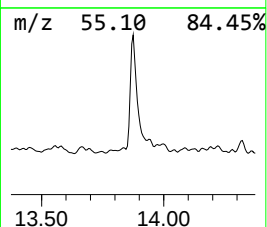
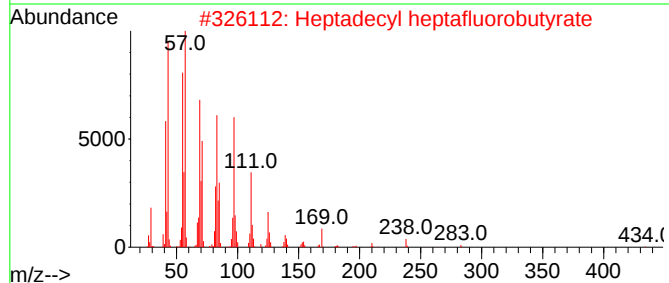
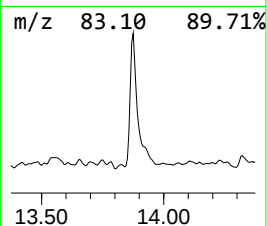
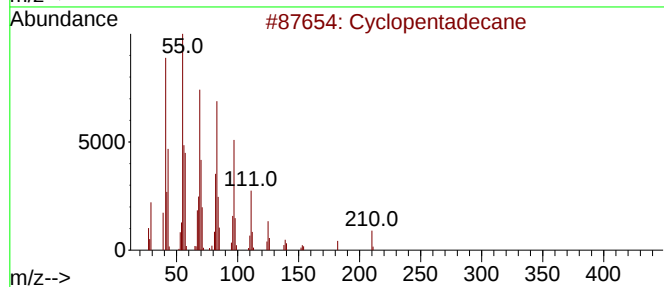
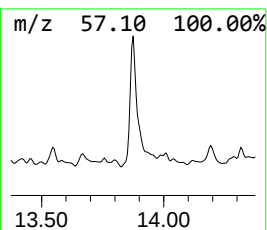
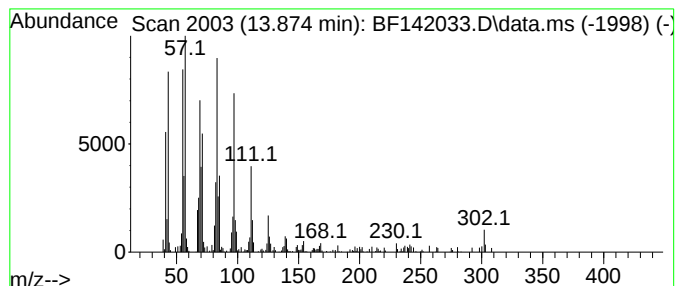
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Cyclopentadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	5.00 ng	209281	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentadecane	210	C15H30	000295-48-7	98
2			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	95
3			2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
4			1-Docosene	308	C22H44	001599-67-3	94
5			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032125\
Data File : BF142033.D
Acq On : 21 Mar 2025 16:51
Operator : RC/JU
Sample : Q1619-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4

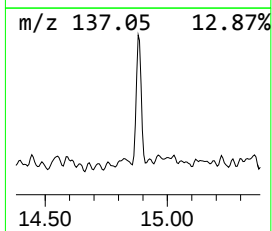
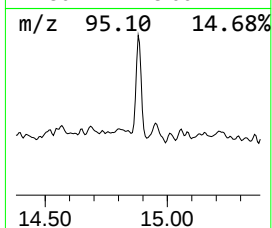
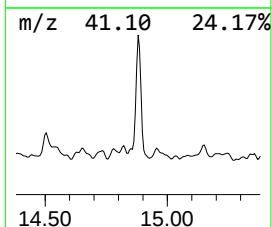
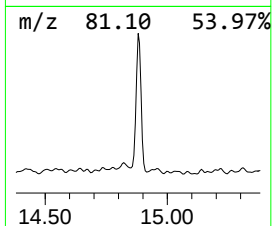
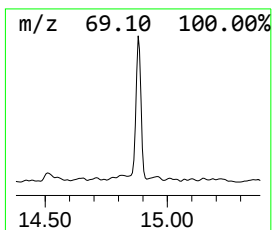
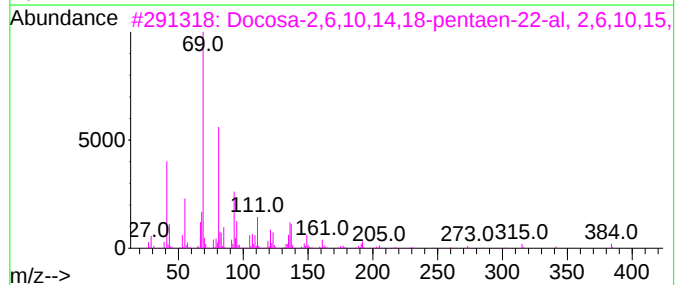
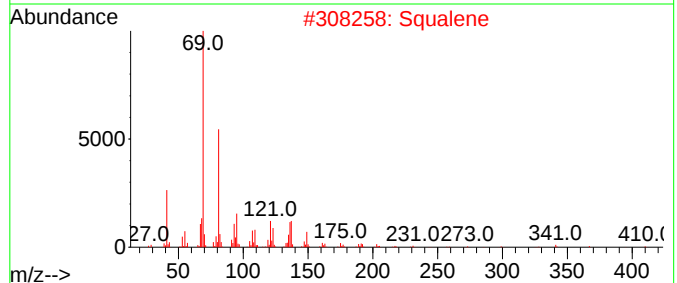
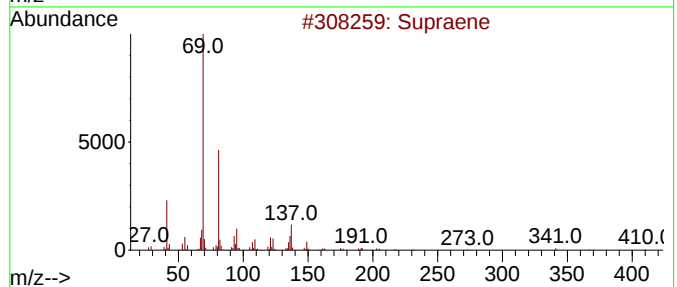
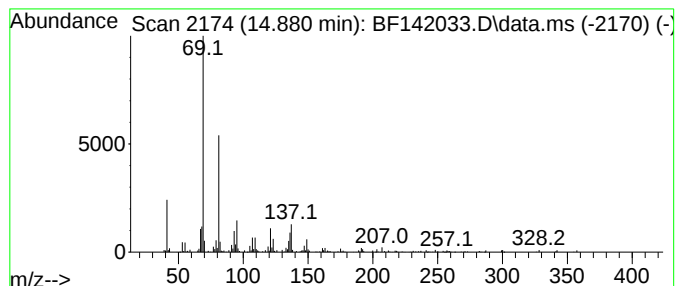
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Supraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.880	2.75 ng	114032	Perylene-d12	15.504

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			Squalene	410	C30H50	000111-02-4	91
3			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	90
4			2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	83
5			2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032125\
Data File : BF142033.D
Acq On : 21 Mar 2025 16:51
Operator : RC/JU
Sample : Q1619-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.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
Butane, 2-metho...	2.163	33.8	ng	1408430	1	6.875	832513	20.0
3-Penten-2-one,...	4.481	6.3	ng	260516	1	6.875	832513	20.0
2-Pentanone, 4-...	5.093	4.4	ng	182498	1	6.875	832513	20.0
Benzophenone	10.622	5.0	ng	327868	3	9.910	1307490	20.0
Cyclopentadecane	13.874	5.0	ng	209281	5	14.033	836290	20.0
Supraene	14.880	2.8	ng	114032	6	15.504	829035	20.0