

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082318\
 Data File : BF108435.D
 Acq On : 23 Aug 2018 21:54
 Operator : JU/SJ
 Sample : J4535-12
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RA-081618-FL-044

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 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-BF080818.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.384	3	8	16	rVB	450256	637292	15.26%	1.819%
2	5.254	491	496	503	rBV	135794	196680	4.71%	0.561%
3	5.631	553	560	563	rBV	3481171	3580039	85.70%	10.221%
4	6.625	722	729	732	rBV	3523249	3775064	90.37%	10.777%
5	6.772	749	754	757	rBV	3883645	3755347	89.90%	10.721%
6	6.819	759	762	766	rVB	66300	52745	1.26%	0.151%
7	6.995	789	792	796	rBV	976325	894050	21.40%	2.552%
8	7.154	815	819	823	rBV	3056948	2920643	69.92%	8.338%
9	7.566	883	889	892	rBV	2343251	2496223	59.76%	7.126%
10	8.284	1006	1011	1014	rBV	1237344	1095571	26.23%	3.128%
11	8.995	1129	1132	1135	rBV	117617	96844	2.32%	0.276%
12	9.095	1144	1149	1152	rBV2	57876	55099	1.32%	0.157%
13	9.284	1174	1181	1184	rBV	58095	62302	1.49%	0.178%
14	9.354	1188	1193	1197	rBV	4141729	4177292	100.00%	11.926%
15	9.419	1202	1204	1208	rVV2	55686	58558	1.40%	0.167%
16	9.619	1234	1238	1242	rBV	65073	97999	2.35%	0.280%
17	9.695	1247	1251	1254	rBV2	63744	71472	1.71%	0.204%
18	9.742	1254	1259	1266	rBV	462139	459650	11.00%	1.312%
19	9.813	1267	1271	1273	rBV2	43929	55925	1.34%	0.160%
20	9.901	1283	1286	1288	rBV2	43121	45560	1.09%	0.130%
21	9.948	1292	1294	1296	rVV	55620	43451	1.04%	0.124%
22	10.042	1304	1310	1314	rBV2	1408288	1248594	29.89%	3.565%
23	10.183	1331	1334	1337	rBV5	38405	58946	1.41%	0.168%
24	10.242	1341	1344	1346	rVV4	59996	67496	1.62%	0.193%
25	10.278	1347	1350	1354	rVV4	73121	98907	2.37%	0.282%
26	10.354	1361	1363	1366	rBV2	42084	44755	1.07%	0.128%
27	10.383	1366	1368	1373	rVV2	52989	63619	1.52%	0.182%
28	10.448	1377	1379	1383	rVB	107194	110282	2.64%	0.315%
29	10.672	1414	1417	1420	rVB	247148	231652	5.55%	0.661%
30	10.836	1441	1445	1454	rBV	2441756	2568433	61.49%	7.333%
31	10.942	1458	1463	1466	rBV	423697	494857	11.85%	1.413%
32	11.407	1539	1542	1545	rBV	337499	285418	6.83%	0.815%
33	11.542	1561	1565	1567	rBV	1127563	1028991	24.63%	2.938%
34	13.124	1830	1834	1838	rVB	2648022	2615345	62.61%	7.466%

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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

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35	14.195	2012	2016	2019	rBV	764426	733644	17.56%	2.094%
36	15.748	2276	2280	2286	rVB	549618	749185	17.93%	2.139%

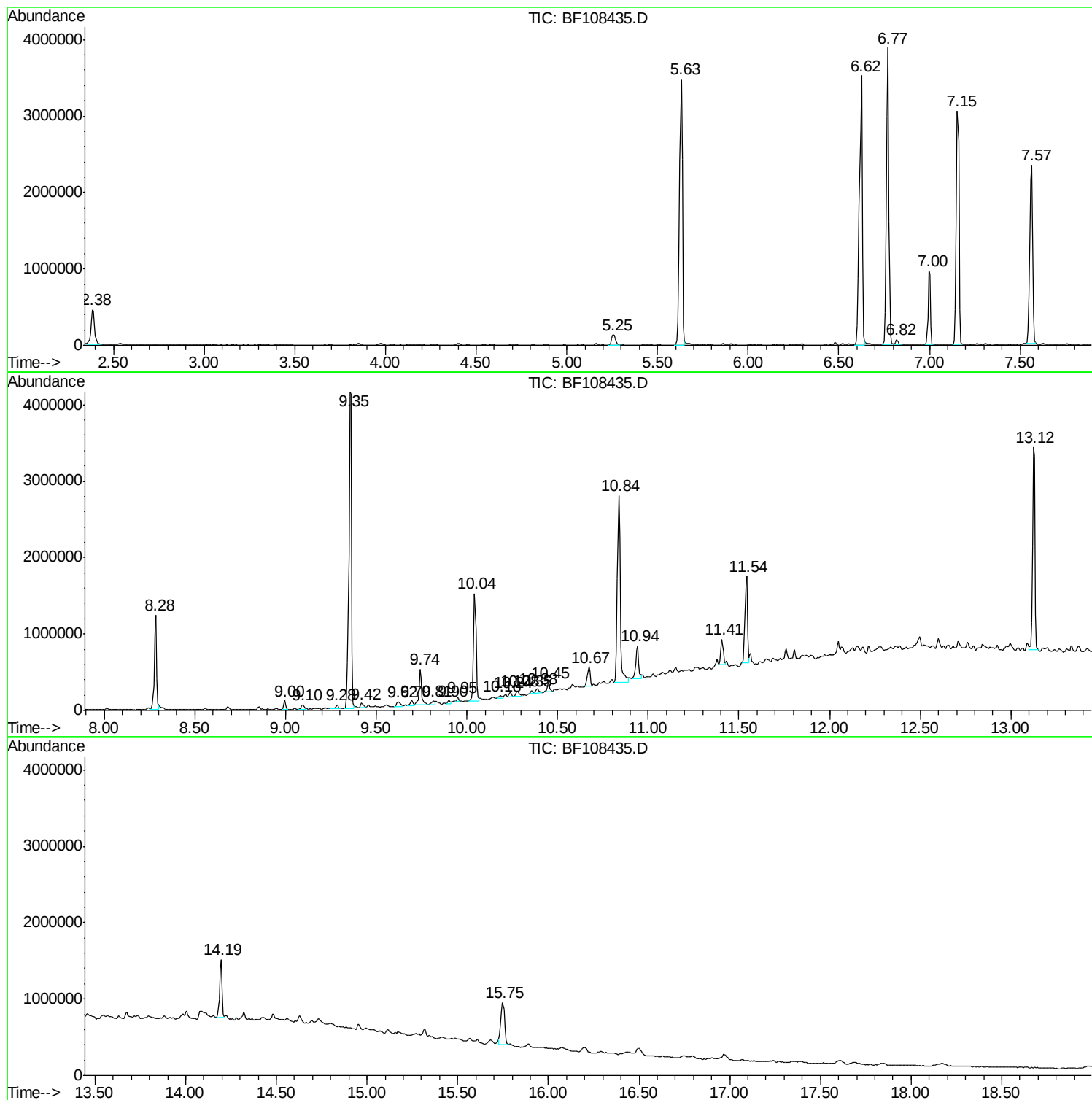
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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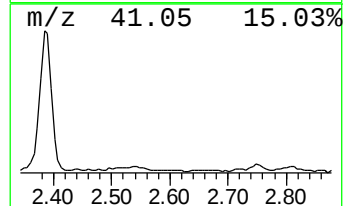
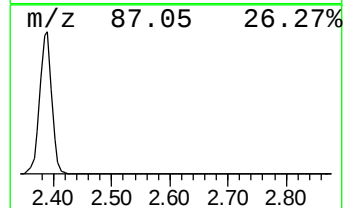
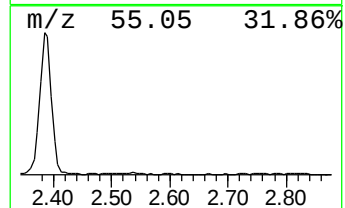
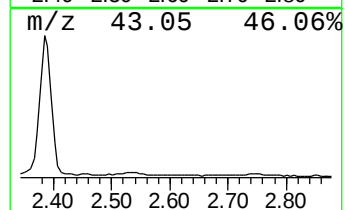
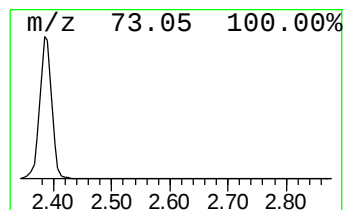
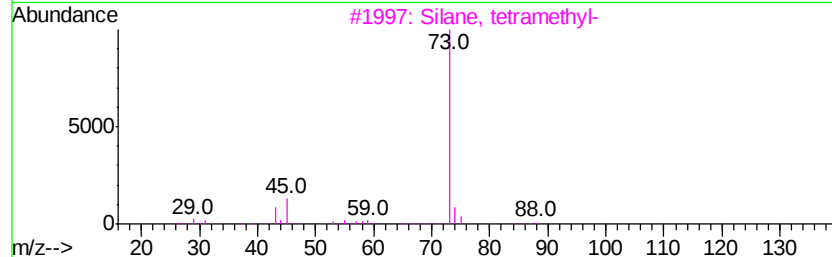
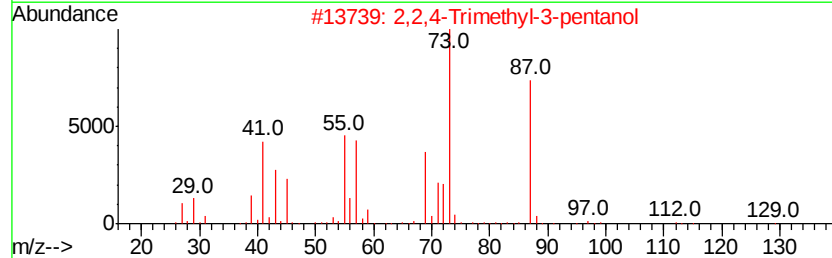
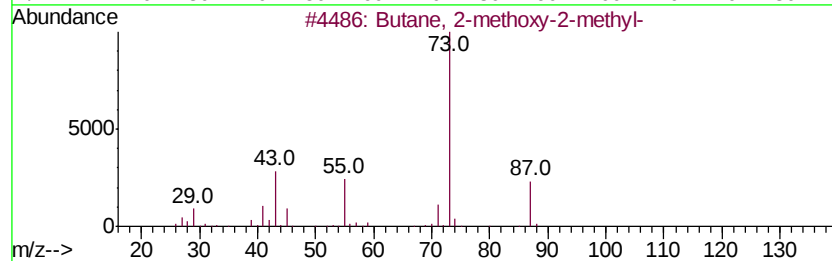
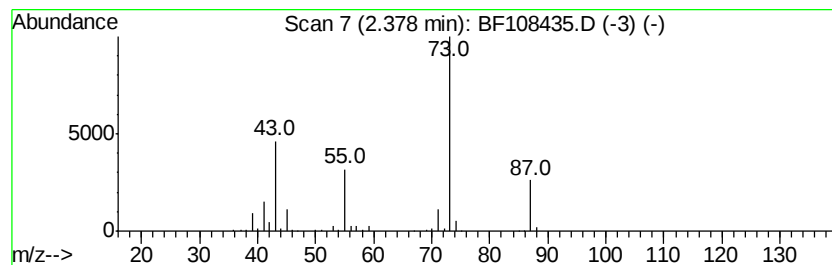
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.38	14.26 ng	637292	1,4-Dichlorobenzene-d4	7.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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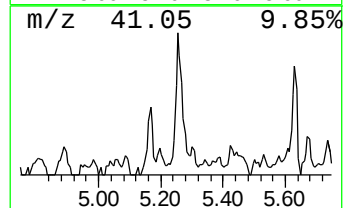
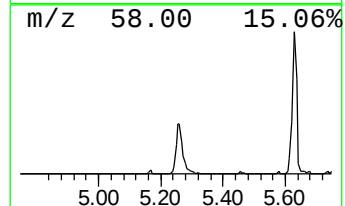
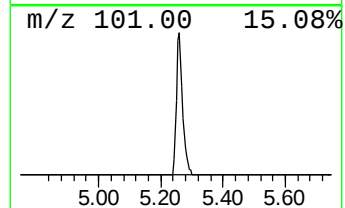
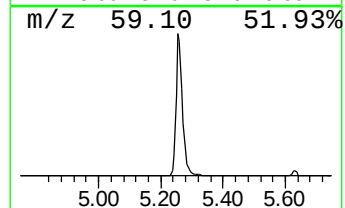
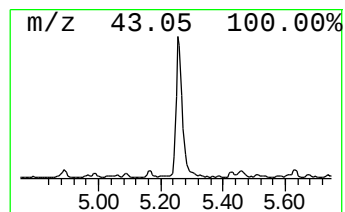
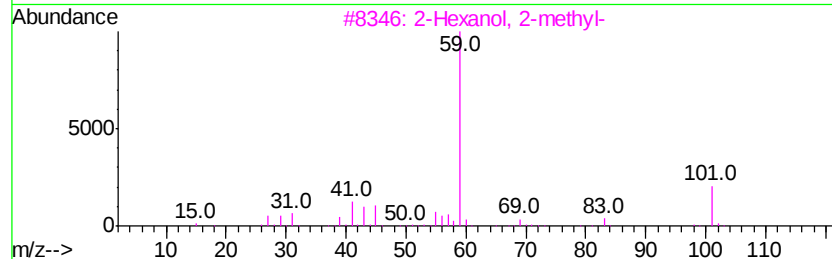
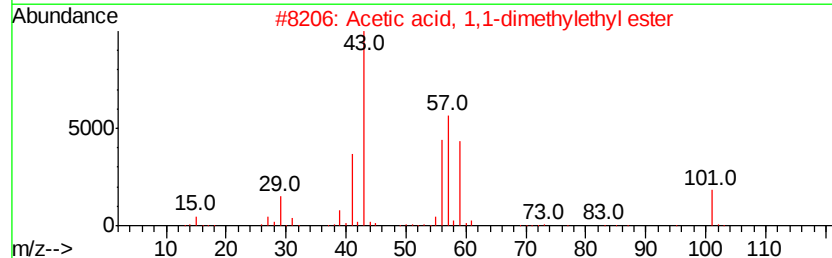
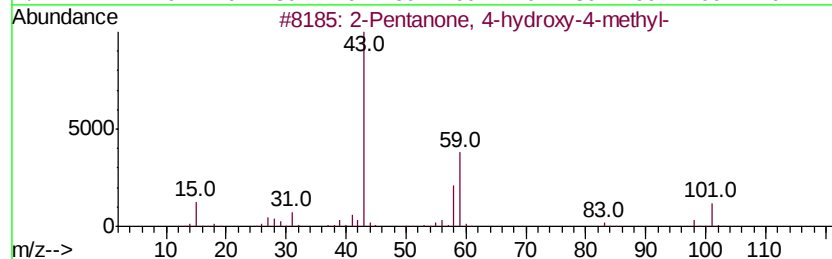
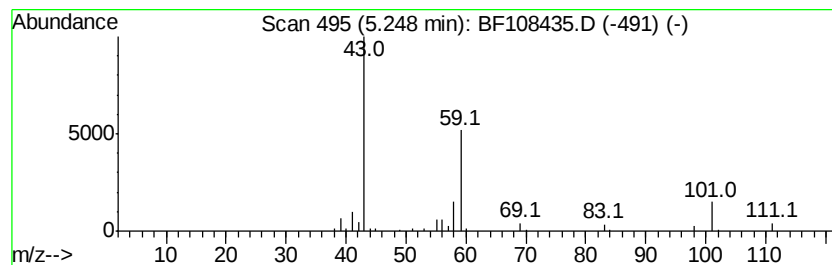
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.25	4.40 ng	196680	1,4-Dichlorobenzene-d4	7.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4		2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	28
5		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17



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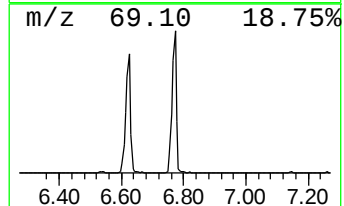
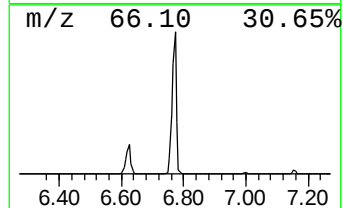
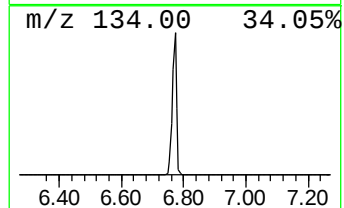
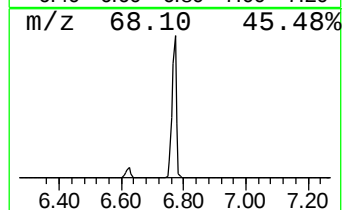
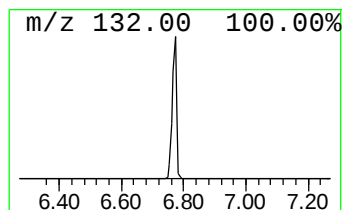
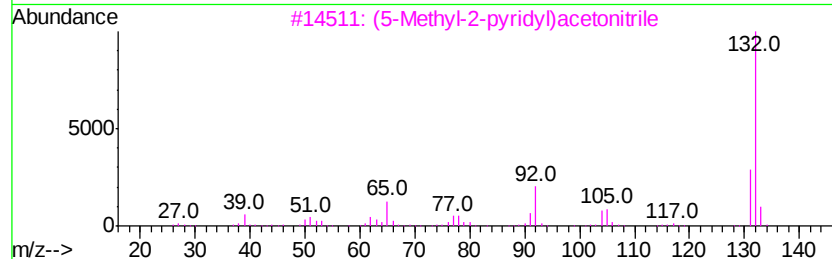
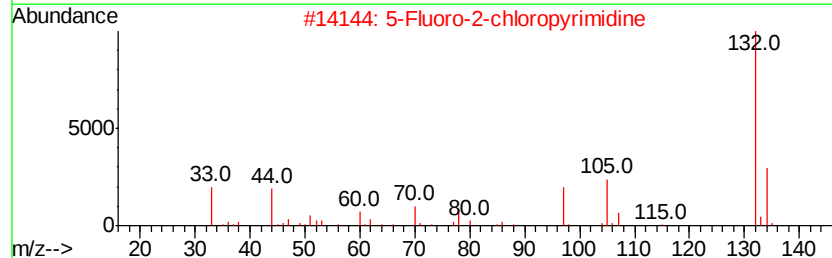
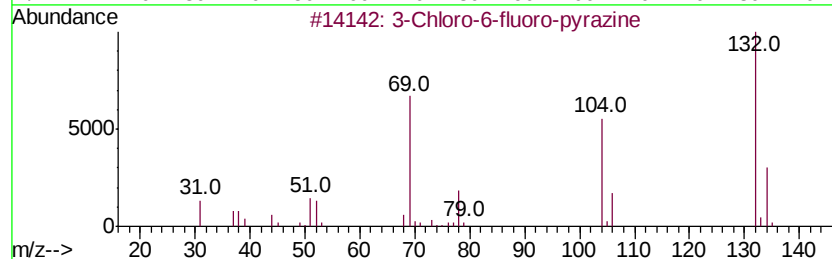
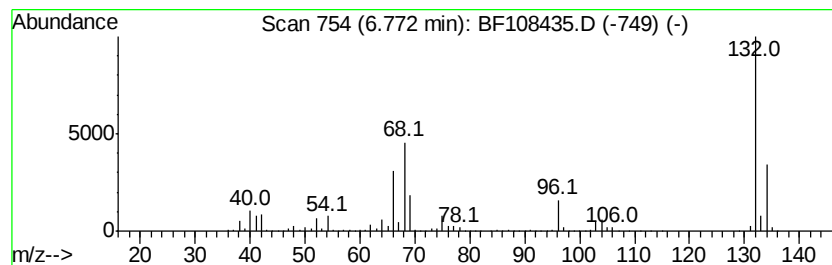
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 unknown6.77 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.77	84.01 ng	3755350	1,4-Dichlorobenzene-d4	7.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	9
5		Xenon	132	Xe	007440-63-3	9



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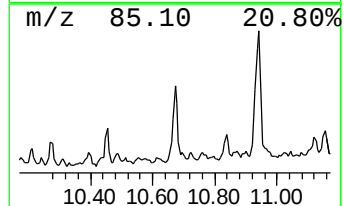
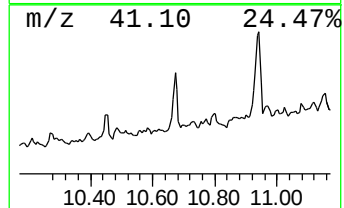
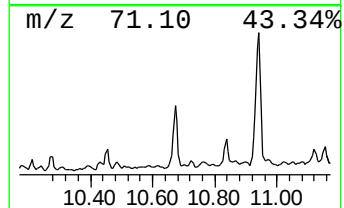
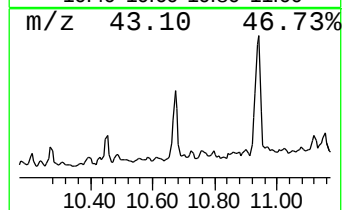
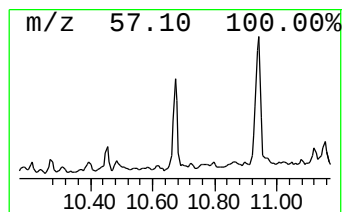
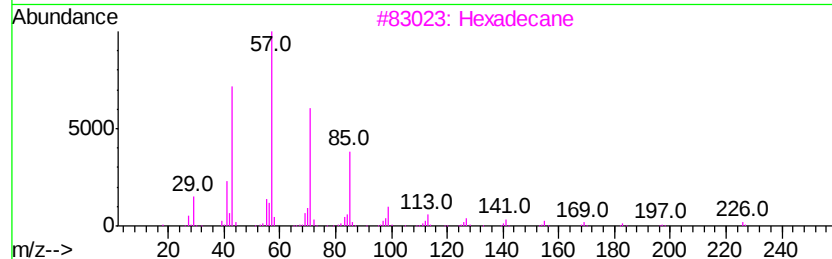
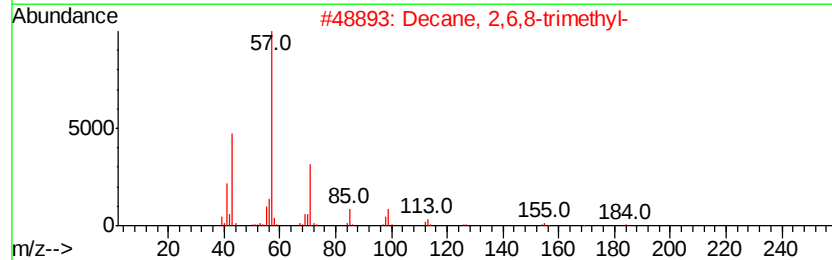
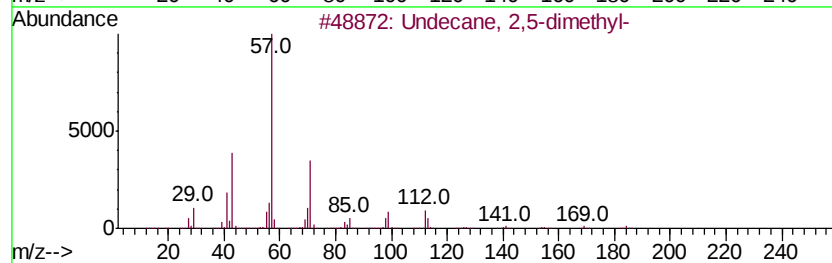
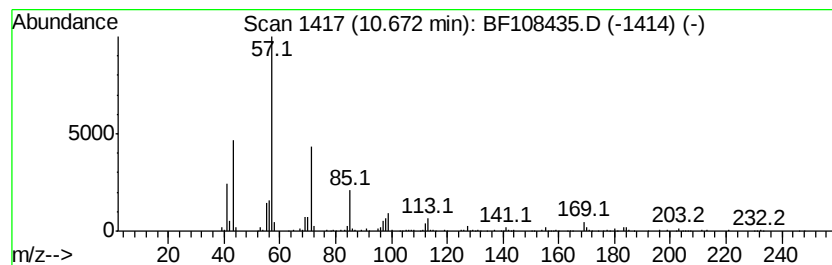
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Undecane, 2,5-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.67	3.71 ng	231652	Acenaphthene-d10		10.04

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 2,5-dimethyl-	184	C13H28	017301-22-3	76
2			Decane, 2,6,8-trimethyl-	184	C13H28	062108-26-3	76
3			Hexadecane	226	C16H34	000544-76-3	64
4			Undecane, 3,9-dimethyl-	184	C13H28	017301-31-4	64
5			Heptacosane	380	C27H56	000593-49-7	64



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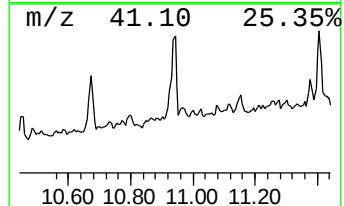
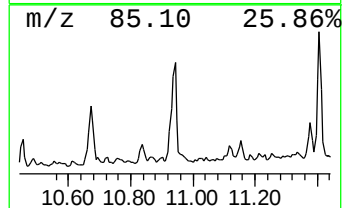
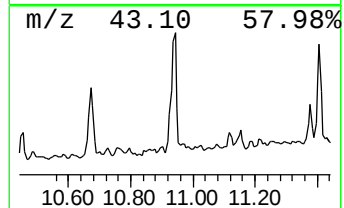
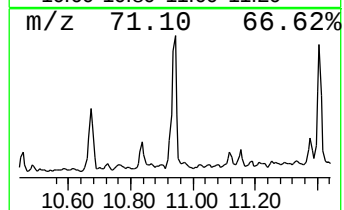
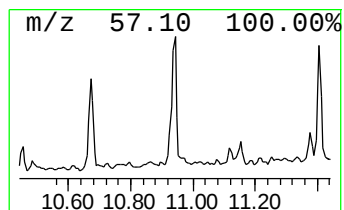
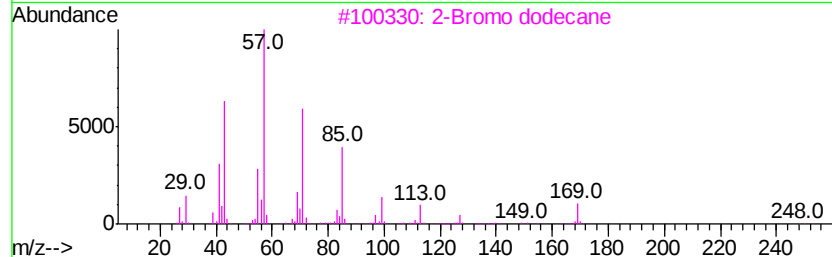
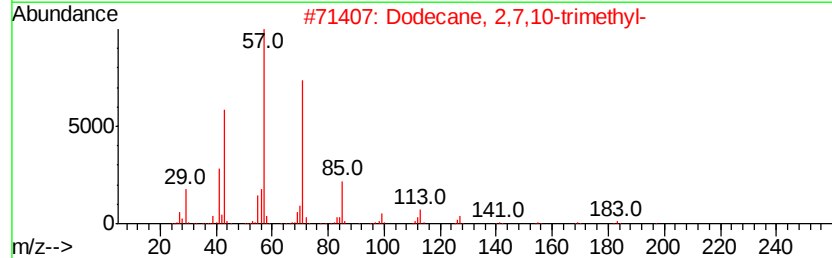
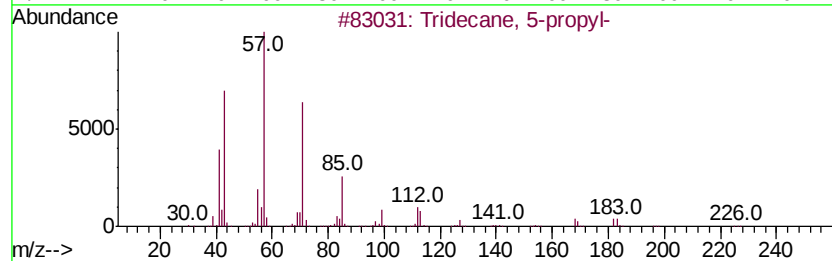
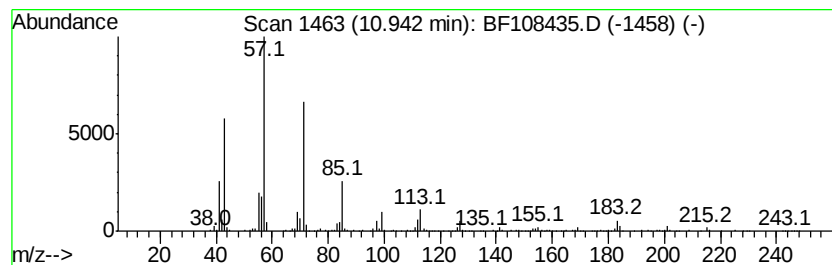
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TIC Integration Parameters: LSCINT.P

Peak Number 6 Tridecane, 5-propyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.94	9.62 ng	494857	Phenanthrene-d10		11.54
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 5-propyl-	226	C16H34	055045-11-9	86
2	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	80
3	2-Bromo dodecane	248	C12H25Br	013187-99-0	78
4	Decane, 2-methyl-	156	C11H24	006975-98-0	72
5	Tridecane	184	C13H28	000629-50-5	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082318\
Data File : BF108435.D
Acq On : 23 Aug 2018 21:54
Operator : JU/SJ
Sample : J4535-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RA-081618-FL-044

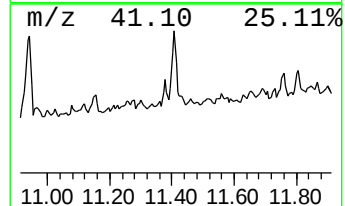
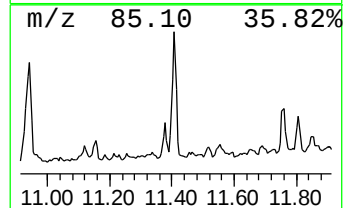
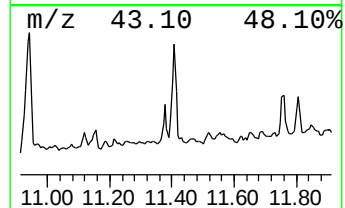
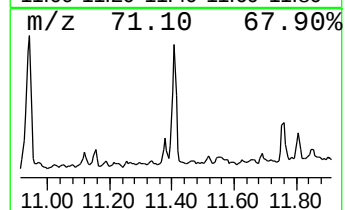
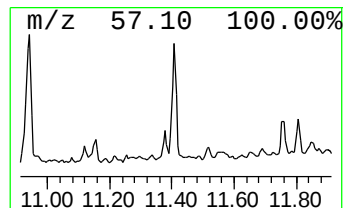
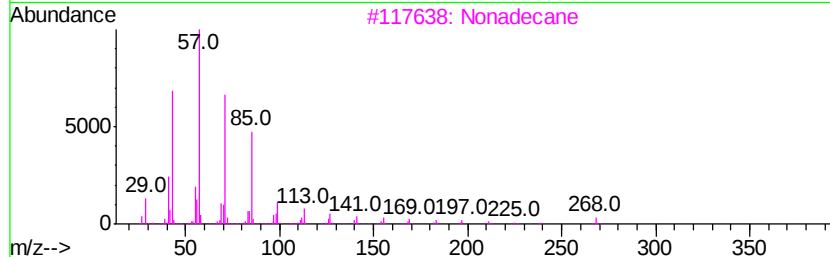
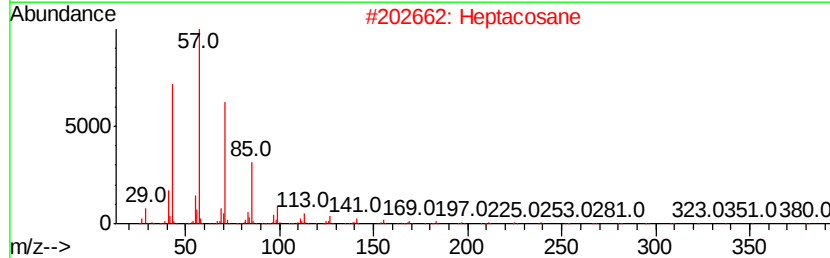
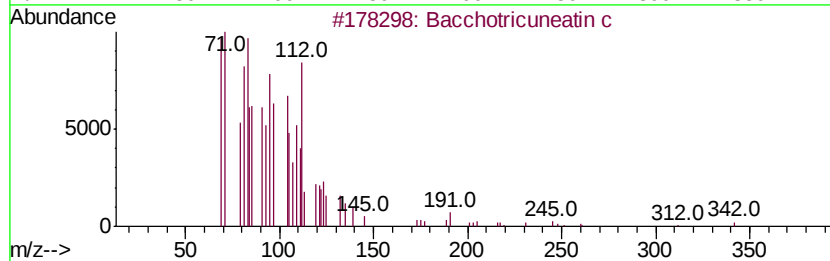
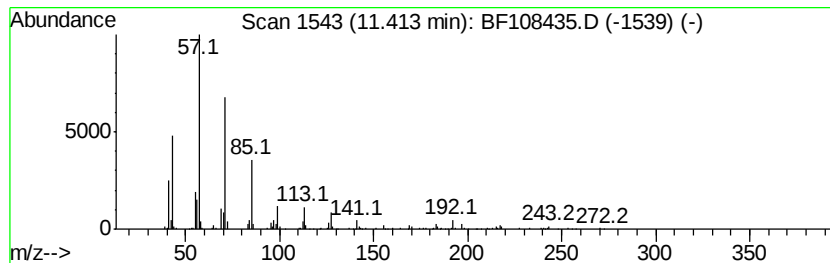
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Bacchotricuneatin c Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.41	5.55 ng	285418	Phenanthrene-d10	11.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bacchotricuneatin c	342	C20H22O5	066563-30-2	95
2	Heptacosane	380	C27H56	000593-49-7	91
3	Nonadecane	268	C19H40	000629-92-5	91
4	Octadecane	254	C18H38	000593-45-3	90
5	Heptadecane	240	C17H36	000629-78-7	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082318\
Data File : BF108435.D
Acq On : 23 Aug 2018 21:54
Operator : JU/SJ
Sample : J4535-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RA-081618-FL-044

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.38	14.3	ng	637292	1	7.00	894050	20.0
2-Pentanone, 4-hy...	5.25	4.4	ng	196680	1	7.00	894050	20.0
unknown6.77	6.77	84.0	ng	3755350	1	7.00	894050	20.0
Undecane, 2,5-dim...	10.67	3.7	ng	231652	3	10.04	1248590	20.0
Tridecane, 5-propyl-	10.94	9.6	ng	494857	4	11.54	1028990	20.0
Bacchotricuneatin c	11.41	5.5	ng	285418	4	11.54	1028990	20.0