

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122021\
 Data File : BF126275.D
 Acq On : 20 Dec 2021 13:31
 Operator : JU/CG
 Sample : M5124-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 F2337-STOPJOINT-TP

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-BF121521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126275.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.116	3	5	11	rVB	605934	643429	14.60%	2.023%
2	2.222	18	23	36	rVB	92457	138138	3.13%	0.434%
3	3.887	301	306	312	rVB	46682	63059	1.43%	0.198%
4	5.034	493	501	512	rBV	1277213	1776930	40.32%	5.586%
5	5.434	563	569	572	rBV	4173879	4383099	99.47%	13.778%
6	5.834	633	637	644	rVB	214474	192246	4.36%	0.604%
7	6.445	735	741	757	rBV	3610615	4406533	100.00%	13.852%
8	6.816	800	804	807	rBV	1371116	1067248	24.22%	3.355%
9	7.375	894	899	902	rBV	2775023	2941387	66.75%	9.246%
10	8.098	1017	1022	1025	rBV	1689057	1422640	32.28%	4.472%
11	9.175	1200	1205	1208	rBV	4152301	3893849	88.37%	12.240%
12	9.263	1216	1220	1225	rVB	112897	109984	2.50%	0.346%
13	9.792	1304	1310	1314	rVB	48609	47403	1.08%	0.149%
14	9.851	1316	1320	1331	rVB	1515911	1327150	30.12%	4.172%
15	10.639	1449	1454	1463	rBV	1902424	1933079	43.87%	6.077%
16	11.298	1561	1566	1569	rBV3	55570	60091	1.36%	0.189%
17	11.333	1569	1572	1575	rBV	1245700	1051910	23.87%	3.307%
18	11.863	1660	1662	1667	rBV	98324	104848	2.38%	0.330%
19	12.139	1703	1709	1717	rVB6	42986	69517	1.58%	0.219%
20	12.545	1774	1778	1781	rBV	135547	120842	2.74%	0.380%
21	12.651	1792	1796	1801	rBV2	35927	47401	1.08%	0.149%
22	12.774	1810	1817	1822	rBV	133106	160632	3.65%	0.505%
23	12.827	1823	1826	1831	rVB3	47498	44186	1.00%	0.139%
24	12.921	1838	1842	1845	rBV	2786187	2519829	57.18%	7.921%
25	13.892	2001	2007	2015	rBV3	98423	303597	6.89%	0.954%
26	13.968	2015	2020	2023	rBV	908412	857882	19.47%	2.697%
27	14.063	2032	2036	2042	rBV	240330	268646	6.10%	0.844%
28	14.757	2151	2154	2162	rVB3	27932	49881	1.13%	0.157%
29	14.833	2163	2167	2172	rVB3	41230	55947	1.27%	0.176%
30	14.998	2190	2195	2198	rBV2	87138	150417	3.41%	0.473%
31	15.098	2208	2212	2216	rVB2	43557	57412	1.30%	0.180%
32	15.292	2241	2245	2251	rVB	65460	82508	1.87%	0.259%
33	15.351	2251	2255	2259	rBV	82970	104429	2.37%	0.328%
34	15.415	2261	2266	2272	rBV2	743626	956347	21.70%	3.006%
35	15.892	2344	2347	2353	rBV4	38650	58566	1.33%	0.184%
36	16.392	2428	2432	2446	rVB6	36325	87541	1.99%	0.275%

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Instrument :
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ClientSampleId :
F2337-STOPJOINT-TP

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-BF121521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	16.839	2503	2508	2517	rVB3	44613	91203	2.07%	0.287%
38	16.974	2527	2531	2536	rBV7	20000	44412	1.01%	0.140%
39	17.262	2576	2580	2587	rVB3	37588	73302	1.66%	0.230%
40	17.956	2694	2698	2705	rVB8	21516	44549	1.01%	0.140%

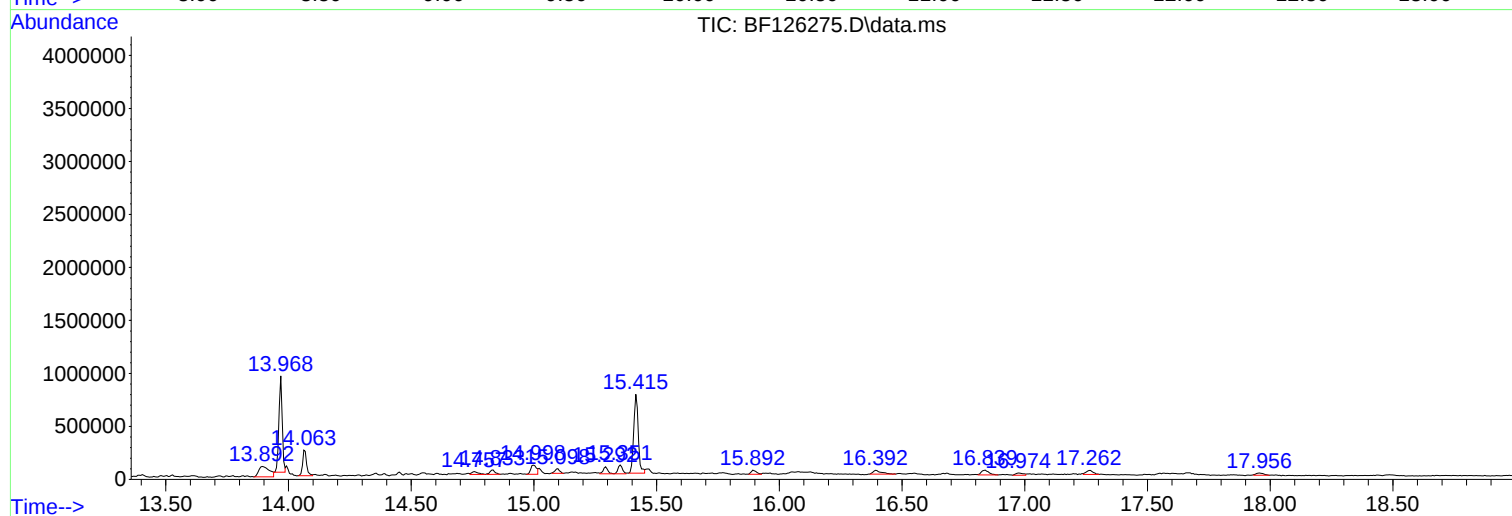
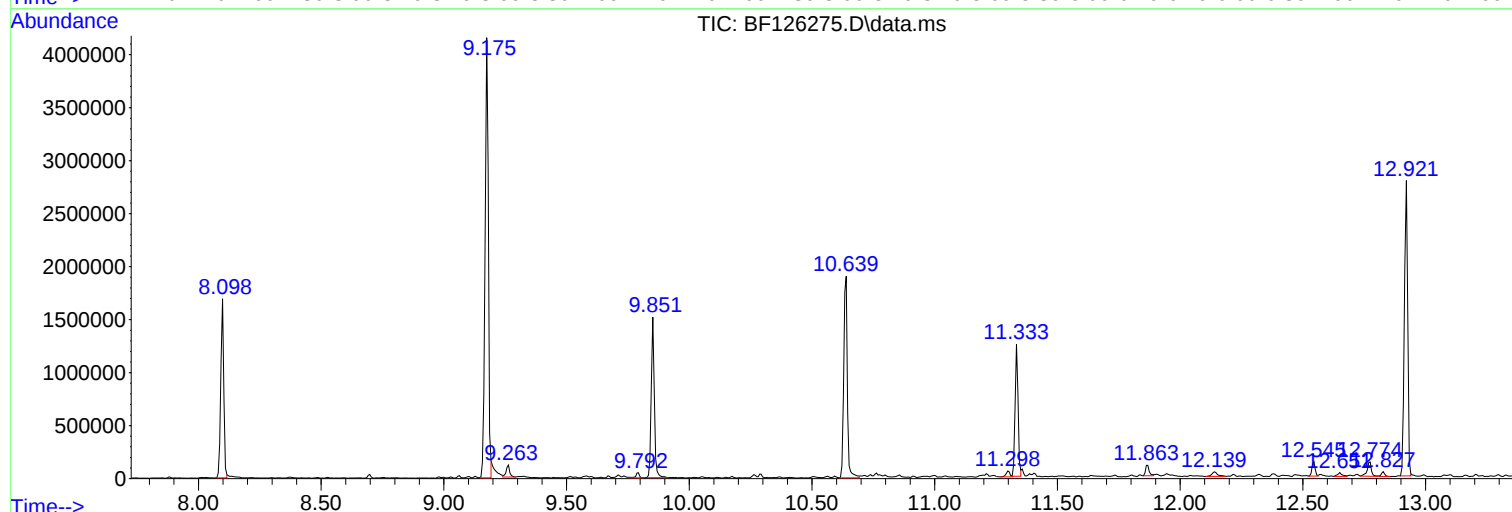
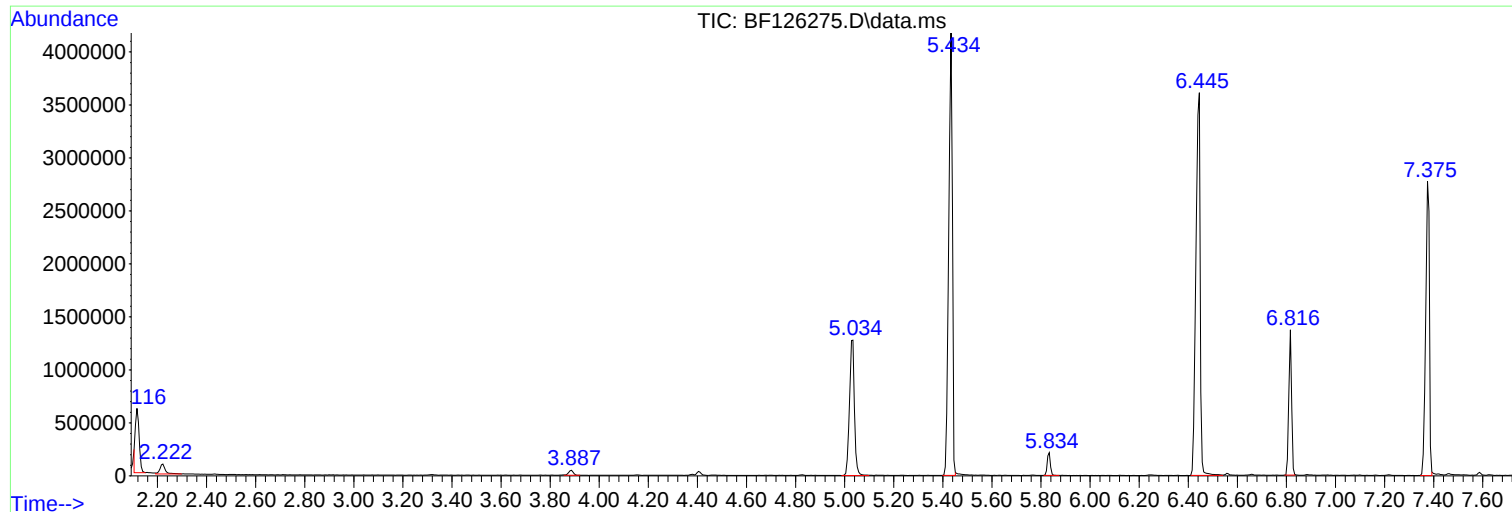
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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F2337-STOPJOINT-TP

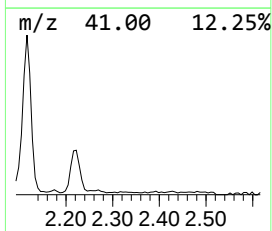
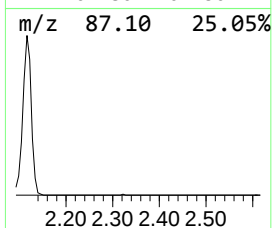
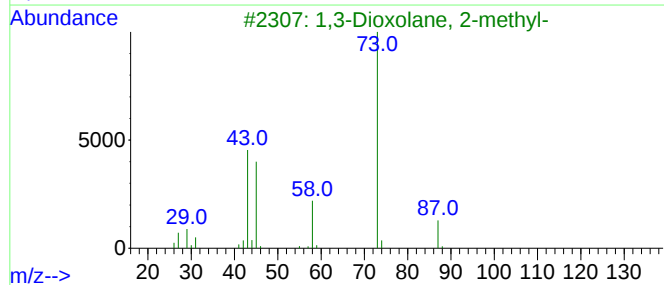
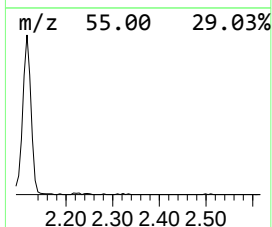
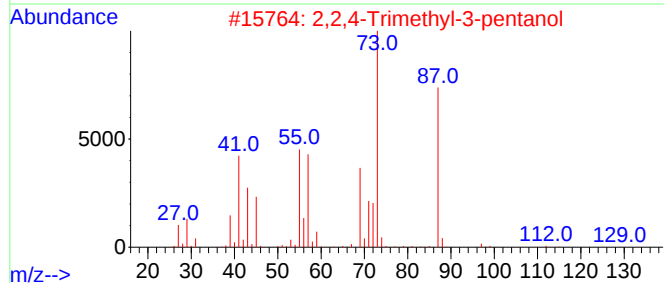
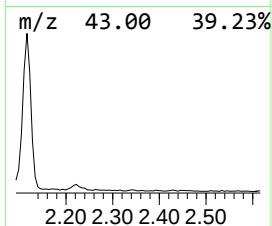
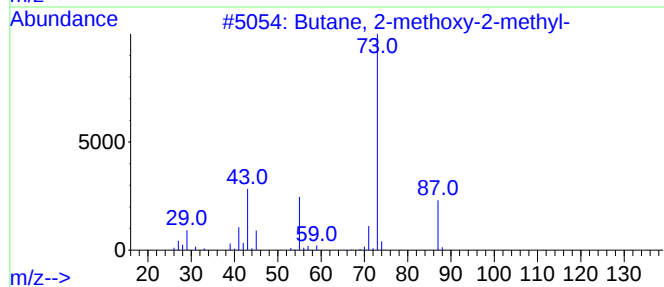
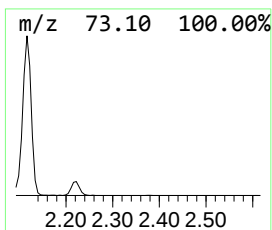
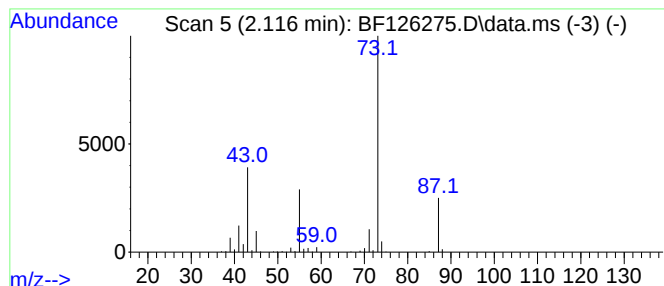
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.116	12.06 ng	643429	1,4-Dichlorobenzene-d4	6.816

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	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
F2337-STOPJOINT-TP

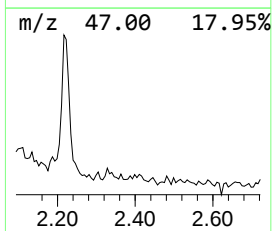
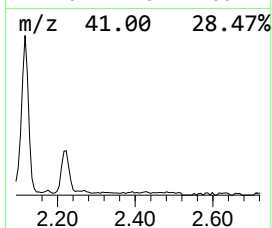
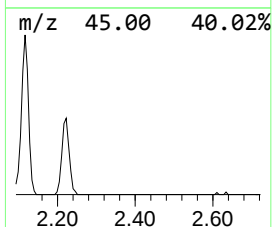
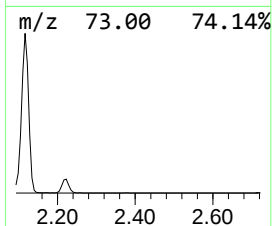
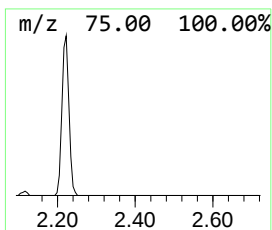
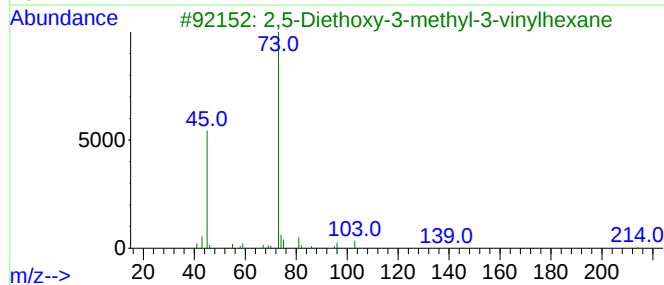
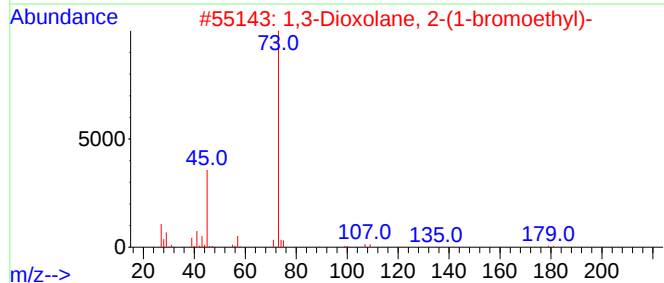
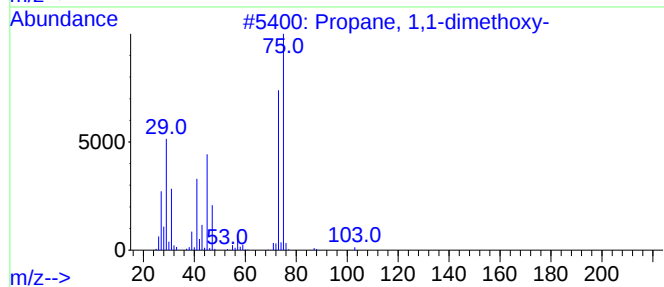
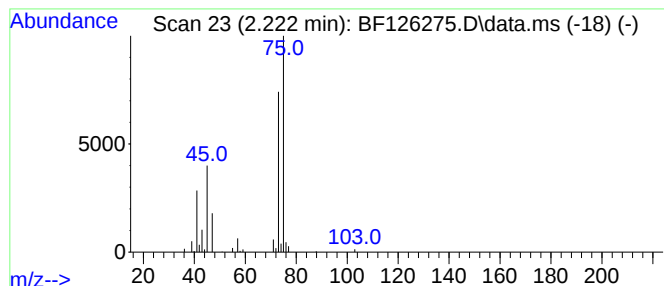
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.222	2.59 ng	138138	1,4-Dichlorobenzene-d4	6.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	78
2			1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	16
3			2,5-Diethoxy-3-methyl-3-vinylhexane	214	C13H26O2	1000432-70-8	9
4			1,3-Dioxolane, 2-(chloromethyl)-	122	C4H7ClO2	002568-30-1	9
5			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	9



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Instrument :
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ClientSampleId :
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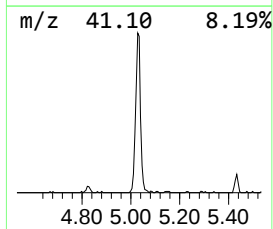
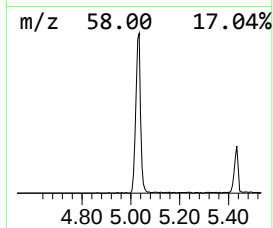
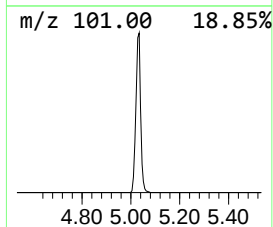
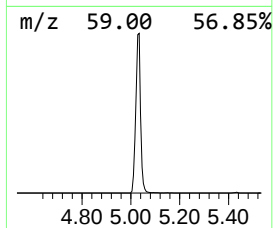
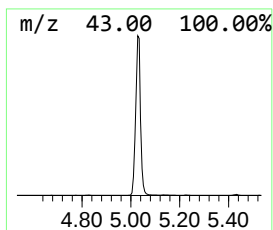
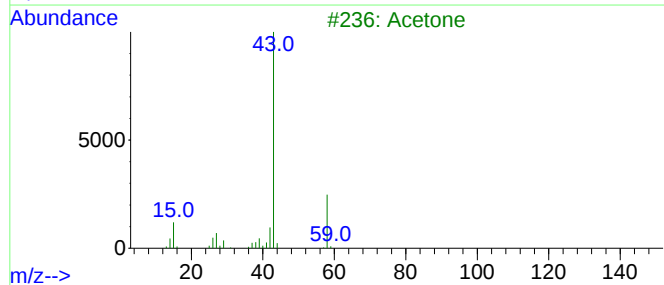
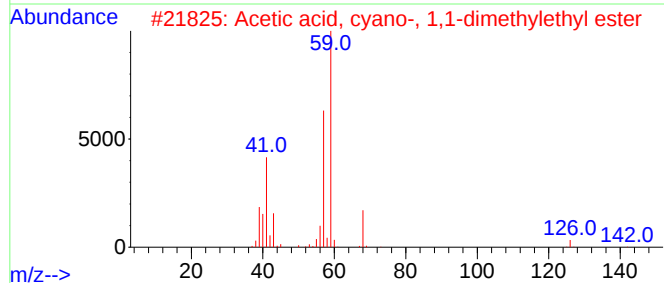
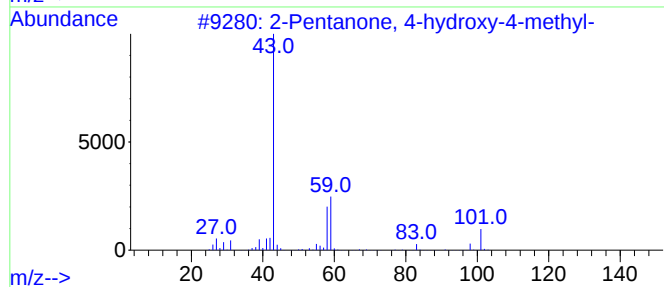
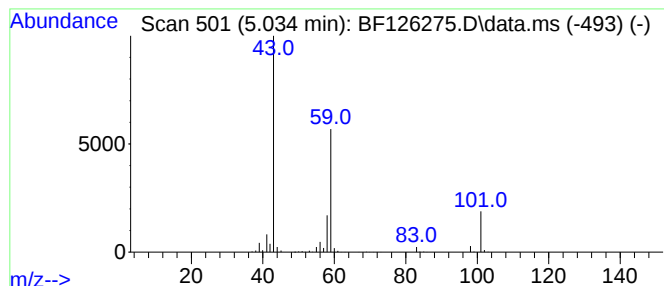
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.034	33.30 ng	1776930	1,4-Dichlorobenzene-d4	6.816

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3		Acetone	58	C3H6O	000067-64-1	9
4		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9
5		Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9



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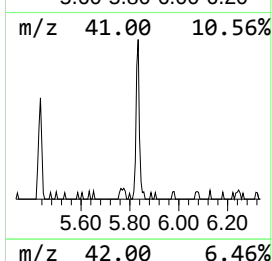
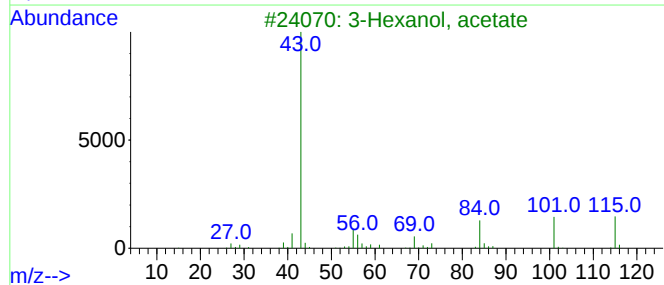
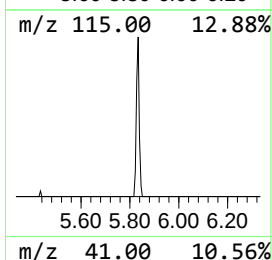
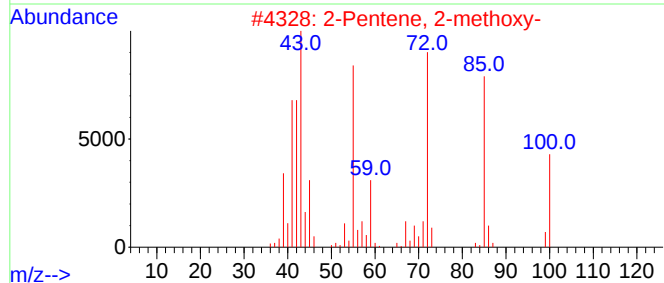
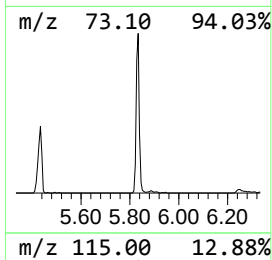
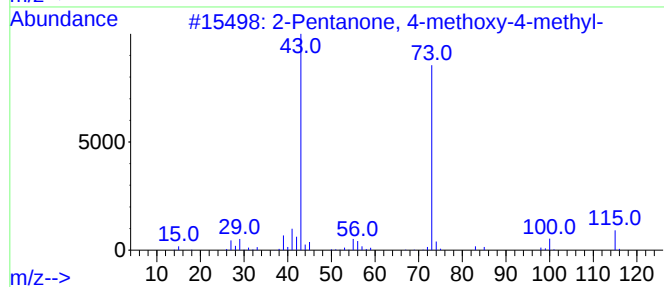
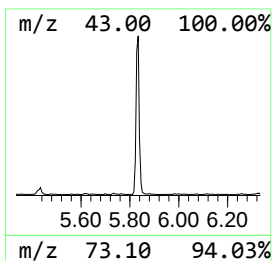
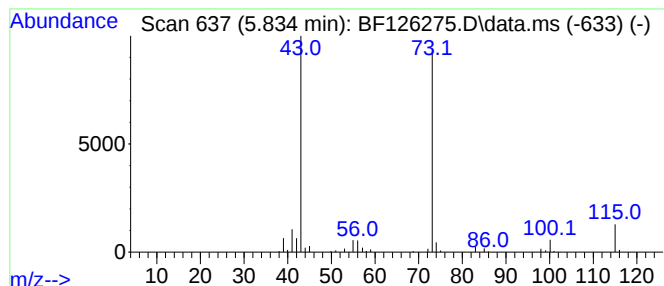
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.834	3.60 ng	192246	1,4-Dichlorobenzene-d4	6.816

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		2-Pentene, 2-methoxy-	100	C6H12O	061142-47-0	12
3		3-Hexanol, acetate	144	C8H16O2	040780-64-1	12
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	10
5		2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9



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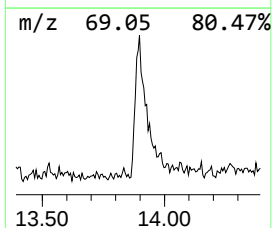
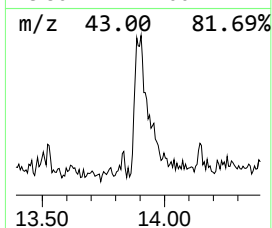
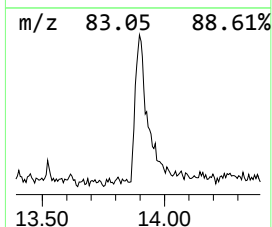
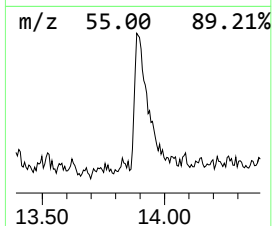
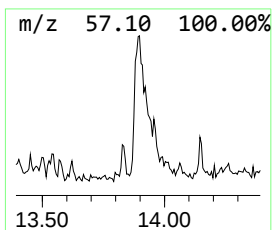
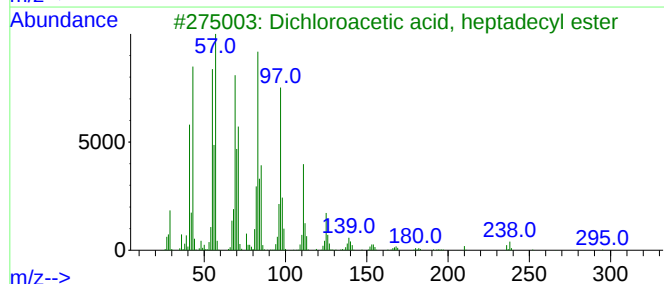
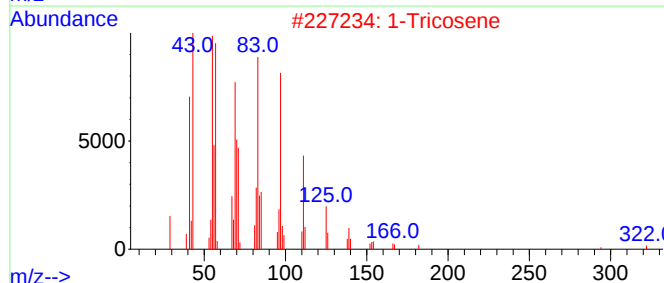
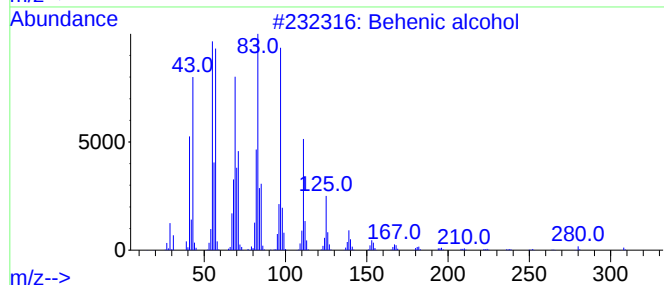
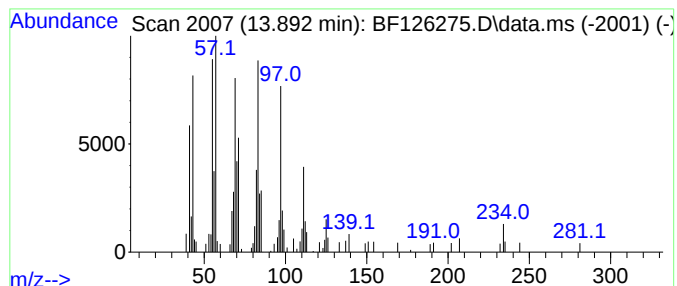
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Behenic alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	7.08 ng	303597	Chrysene-d12	13.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Behenic alcohol	326	C22H46O	000661-19-8	94
2			1-Tricosene	322	C23H46	018835-32-0	93
3			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
4			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
5			n-Tetracosanol-1	354	C24H50O	000506-51-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122021\
Data File : BF126275.D
Acq On : 20 Dec 2021 13:31
Operator : JU/CG
Sample : M5124-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
F2337-STOPJOINT-TP

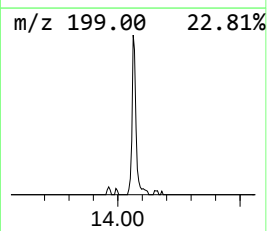
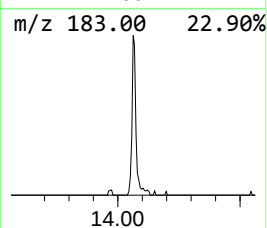
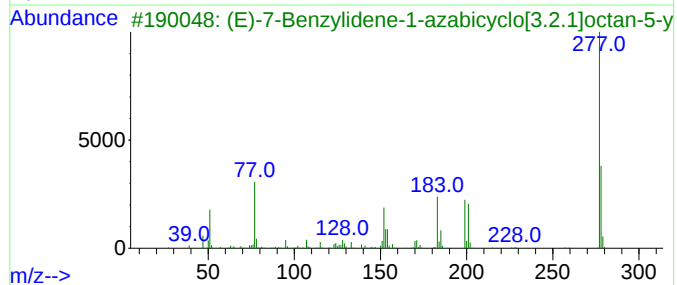
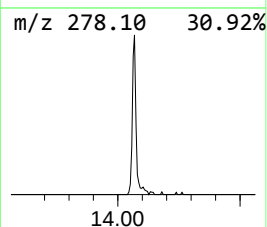
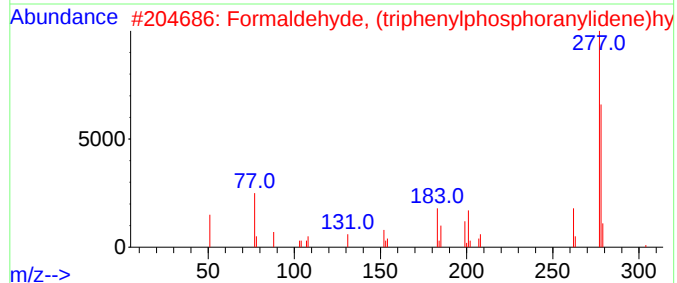
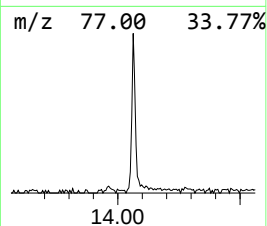
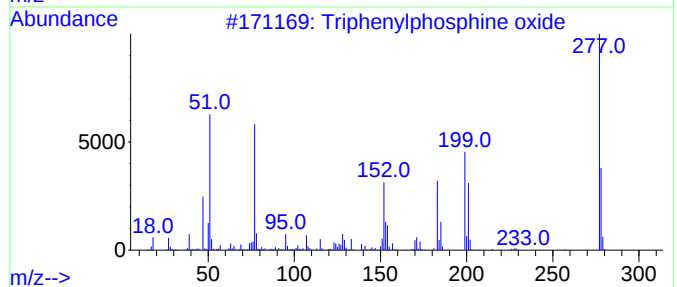
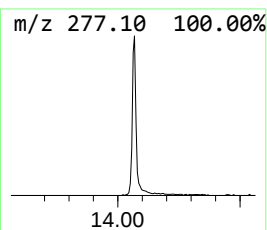
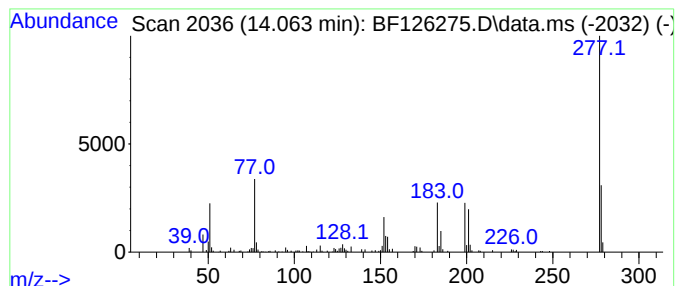
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Triphenylphosphine oxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.063	6.26 ng	268646	Chrysene-d12	13.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50
3			(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	46
4			Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	37
5			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122021\
Data File : BF126275.D
Acq On : 20 Dec 2021 13:31
Operator : JU/CG
Sample : M5124-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
F2337-STOPJOINT-TP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.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...	2.116	12.1	ng	643429	1	6.816	1067250	20.0
Propane, 1,1-di...	2.222	2.6	ng	138138	1	6.816	1067250	20.0
2-Pentanone, 4-...	5.034	33.3	ng	1776930	1	6.816	1067250	20.0
2-Pentanone, 4-...	5.834	3.6	ng	192246	1	6.816	1067250	20.0
Behenic alcohol	13.892	7.1	ng	303597	5	13.968	857882	20.0
Triphenylphosph...	14.063	6.3	ng	268646	5	13.968	857882	20.0