

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120922\
 Data File : BF131580.D
 Acq On : 09 Dec 2022 22:25
 Operator : CG\JU
 Sample : N5965-01
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-P

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-BF120822.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131580.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.199	12	19	25	rVB	331058	429463	24.52%	3.578%
2	5.128	512	517	525	rVB	162281	196177	11.20%	1.635%
3	5.528	580	585	588	rBV	1529192	1404220	80.19%	11.700%
4	6.539	751	757	760	rBV	1454635	1454060	83.03%	12.115%
5	6.910	816	820	823	rBV	475511	414034	23.64%	3.450%
6	7.475	911	916	919	rBV	1015164	916568	52.34%	7.637%
7	8.198	1035	1039	1042	rBV	637363	504205	28.79%	4.201%
8	9.280	1217	1223	1226	rBV	2027555	1751197	100.00%	14.591%
9	9.963	1335	1339	1342	rVB	635158	559638	31.96%	4.663%
10	10.751	1469	1473	1476	rBV	1180182	950221	54.26%	7.917%
11	10.857	1489	1491	1497	rVB3	15873	21525	1.23%	0.179%
12	11.457	1589	1593	1595	rBV	555778	516247	29.48%	4.301%
13	11.474	1595	1596	1602	rVV	57124	50934	2.91%	0.424%
14	11.527	1602	1605	1607	rVB2	22770	23552	1.34%	0.196%
15	11.616	1617	1620	1625	rVB	19939	19597	1.12%	0.163%
16	11.974	1679	1681	1685	rVB2	31164	30319	1.73%	0.253%
17	12.016	1685	1688	1690	rBV	22231	19495	1.11%	0.162%
18	12.068	1694	1697	1700	rBV2	20032	25121	1.43%	0.209%
19	12.668	1796	1799	1803	rBV	87838	79664	4.55%	0.664%
20	12.904	1833	1839	1843	rBV	80941	98990	5.65%	0.825%
21	13.045	1859	1863	1866	rBV	1581557	1254210	71.62%	10.450%
22	13.227	1892	1894	1897	rVB2	19885	20129	1.15%	0.168%
23	13.968	2017	2020	2030	rVB2	19434	45752	2.61%	0.381%
24	14.104	2038	2043	2046	rBV	406019	385585	22.02%	3.213%
25	14.204	2054	2060	2063	rBV	290137	326601	18.65%	2.721%
26	14.874	2171	2174	2179	rBV4	36399	46740	2.67%	0.389%
27	14.968	2187	2190	2193	rVB	72779	71182	4.06%	0.593%
28	15.168	2221	2224	2228	rBV	24376	35675	2.04%	0.297%
29	15.621	2296	2301	2310	rVB	251698	350565	20.02%	2.921%

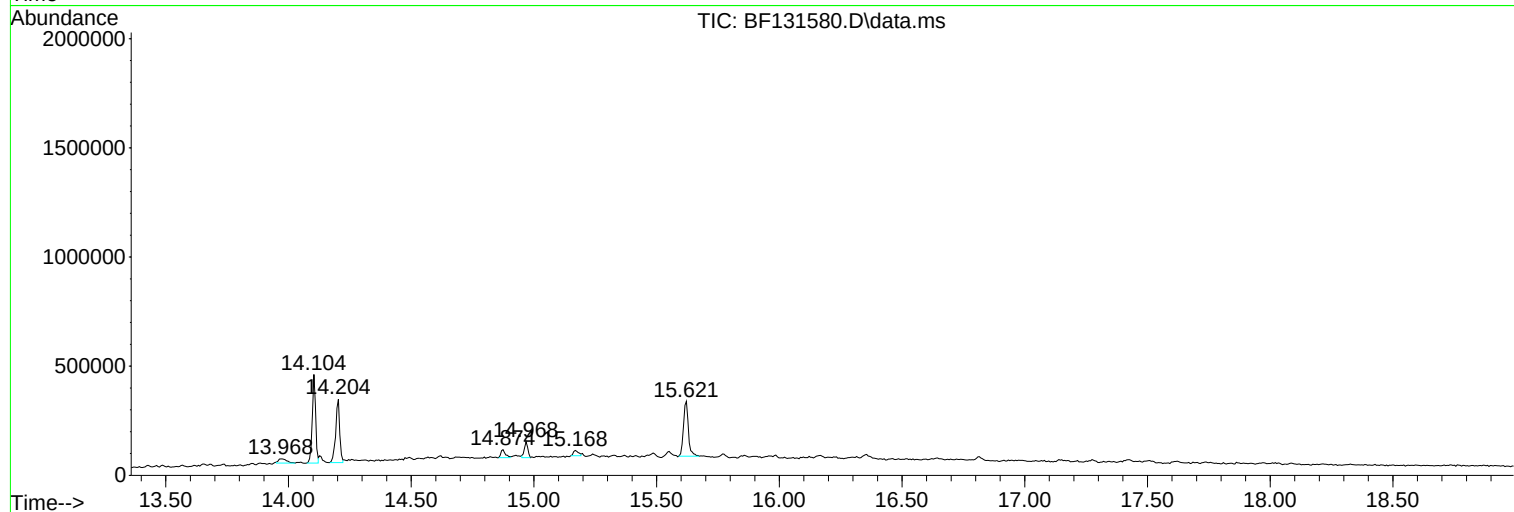
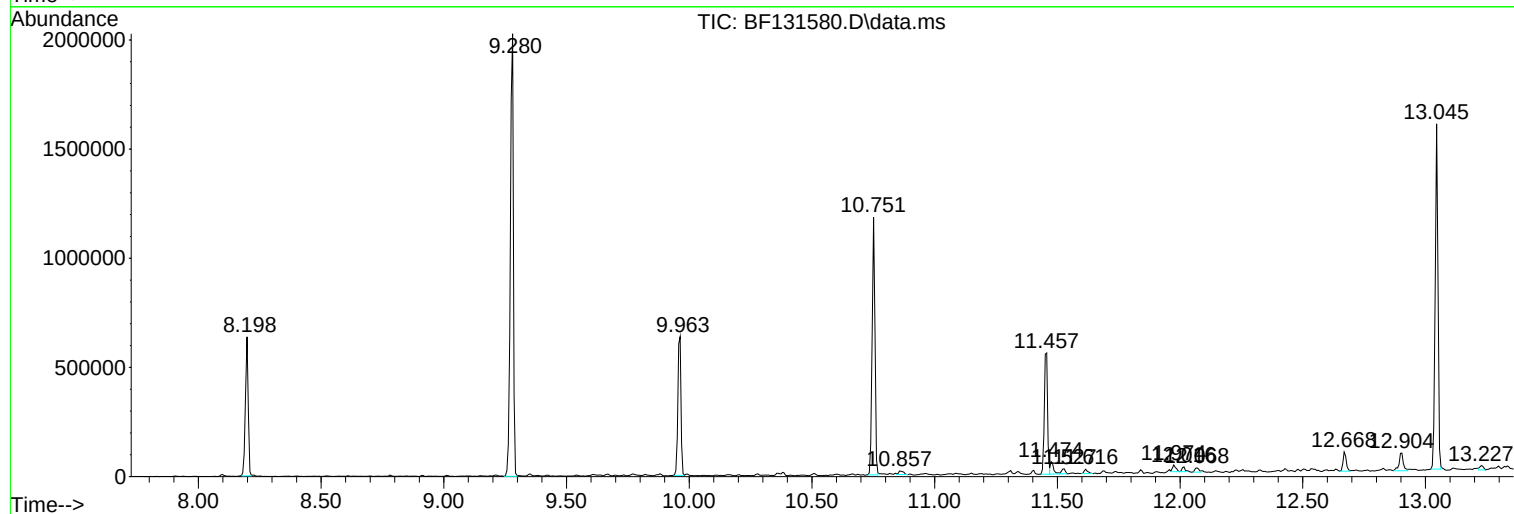
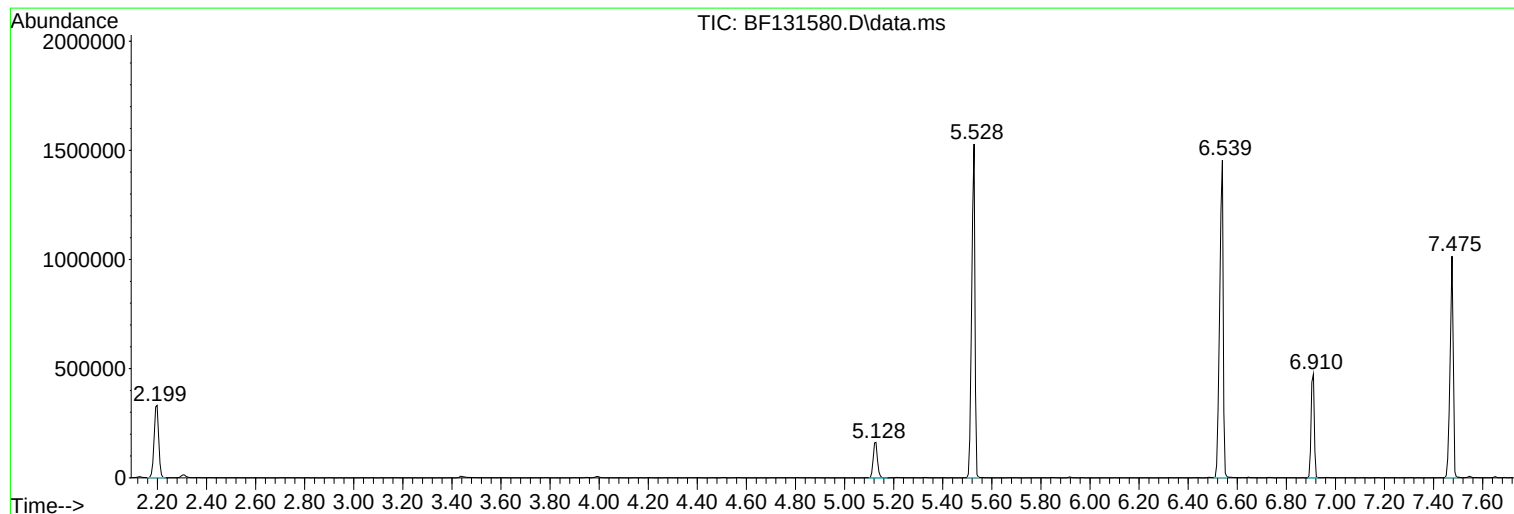
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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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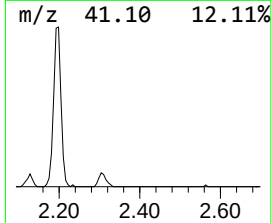
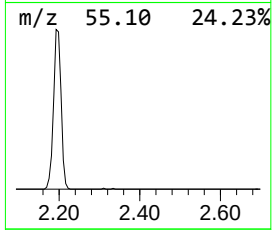
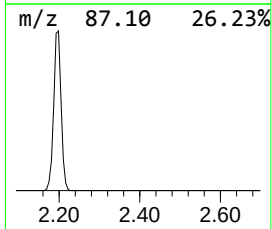
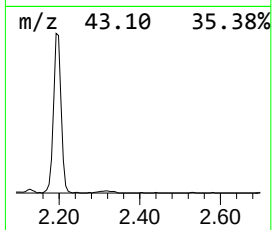
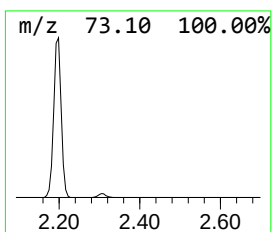
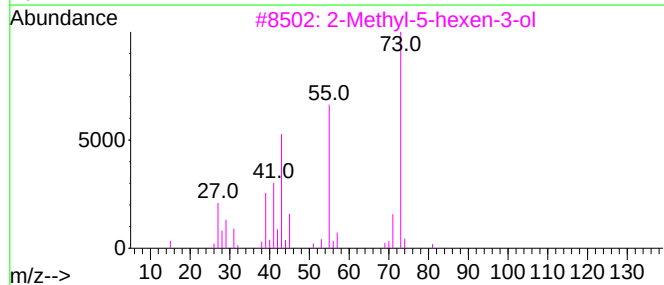
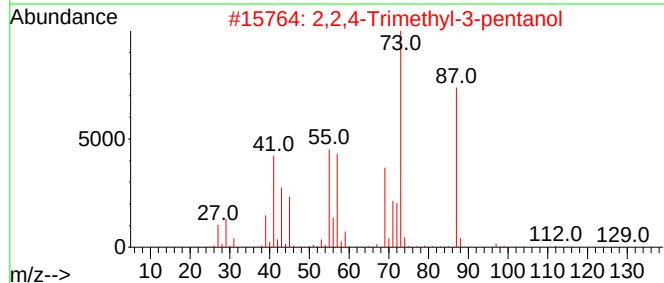
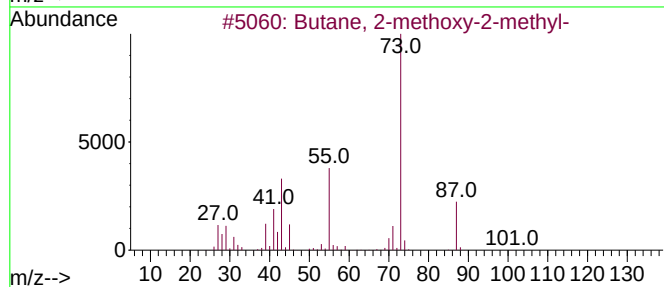
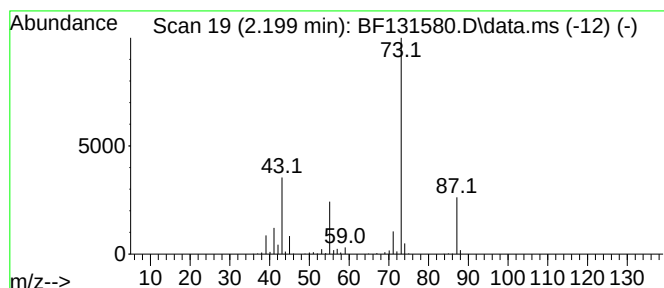
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.199	20.75 ng	429463	1,4-Dichlorobenzene-d4	6.910

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			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	32
4			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	25
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23



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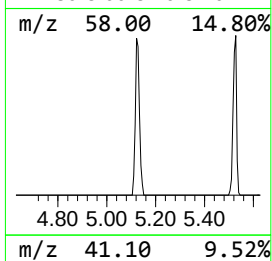
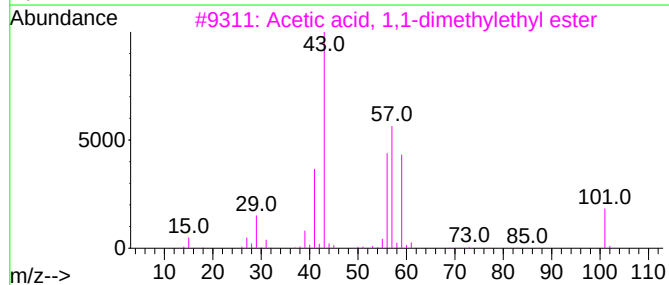
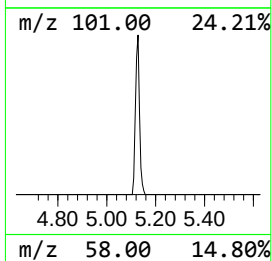
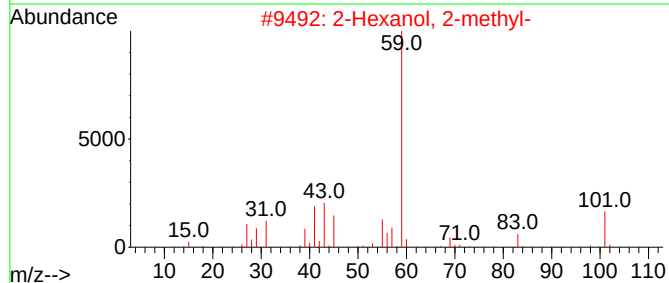
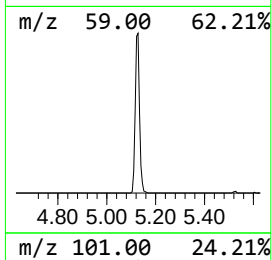
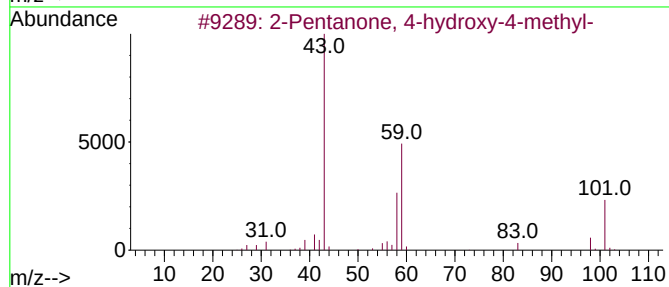
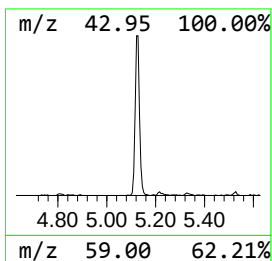
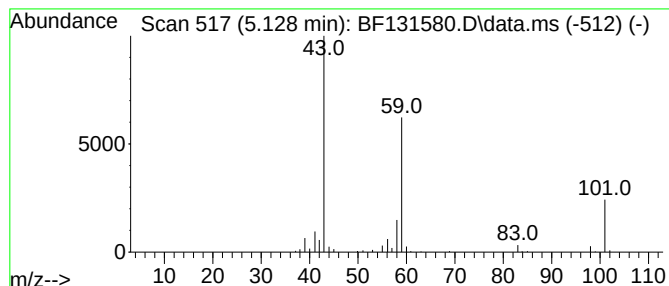
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.128	9.48 ng	196177	1,4-Dichlorobenzene-d4	6.910

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	40
3		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
4		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17
5		Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	17



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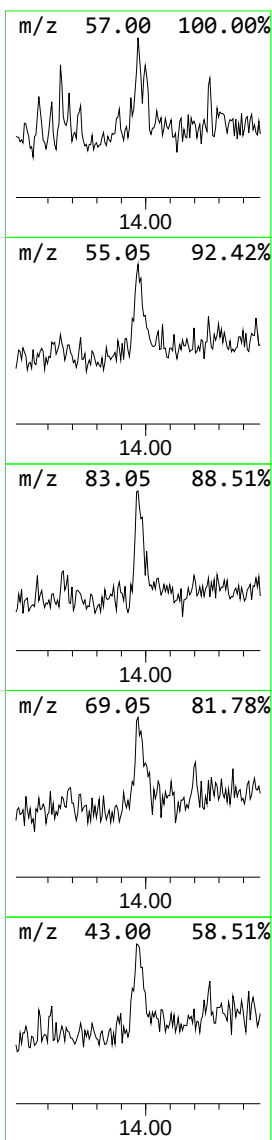
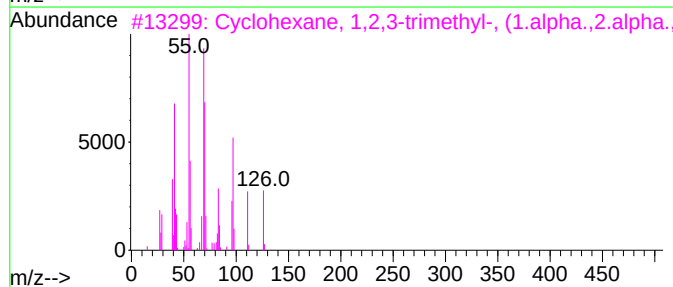
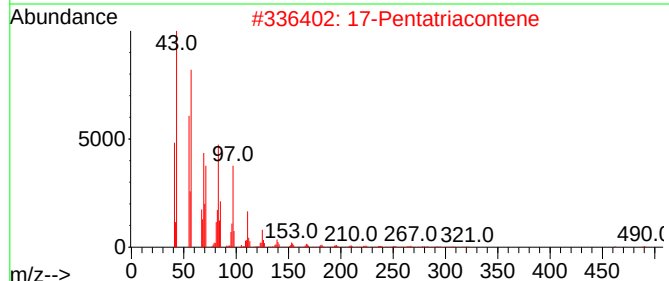
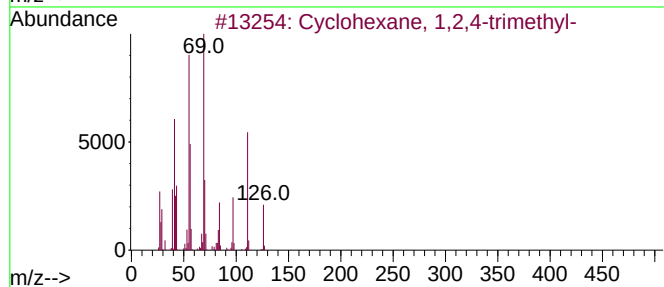
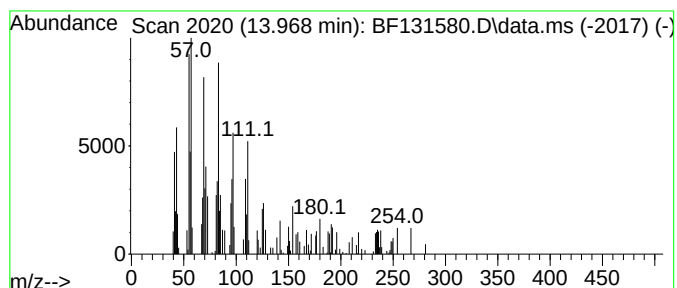
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Cyclohexane, 1,2,4-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.968	2.37 ng	45752	Chrysene-d12	14.104	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,2,4-trimethyl-	126	C9H18	002234-75-5	83
2	17-Pentatriacontene	491	C35H70	006971-40-0	58
3	Cyclohexane, 1,2,3-trimethyl-, (...)	126	C9H18	007667-55-2	50
4	2,3-Dimethyl-3-heptene	126	C9H18	1000113-49-3	49
5	Cyclohexane, 1,2,3-trimethyl-	126	C9H18	001678-97-3	45



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Misc :
ALS Vial : 20 Sample Multiplier: 1

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ClientSampleId :
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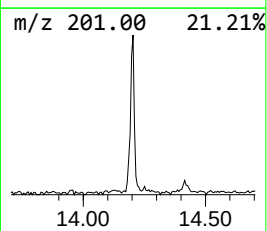
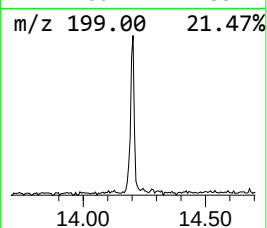
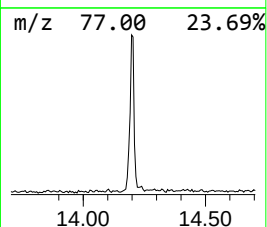
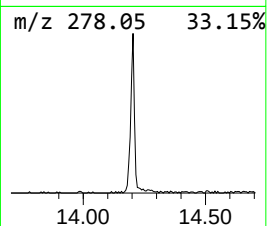
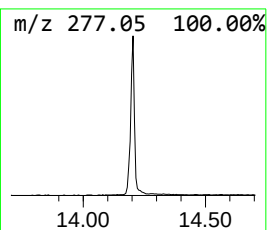
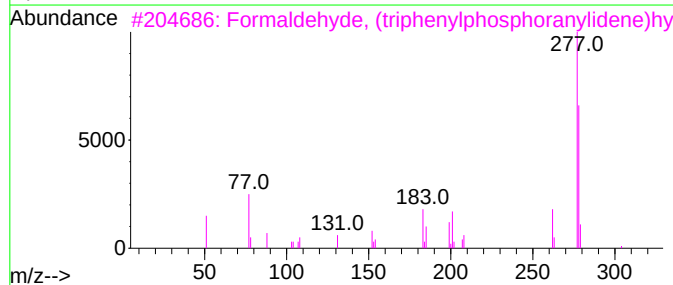
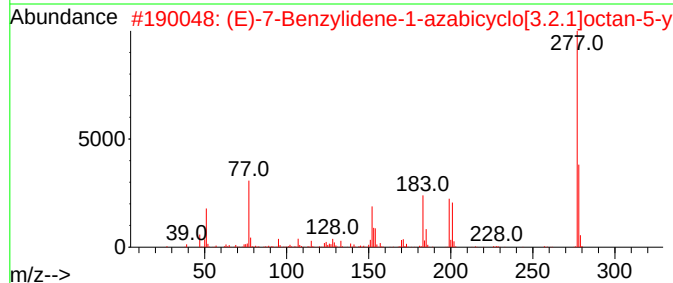
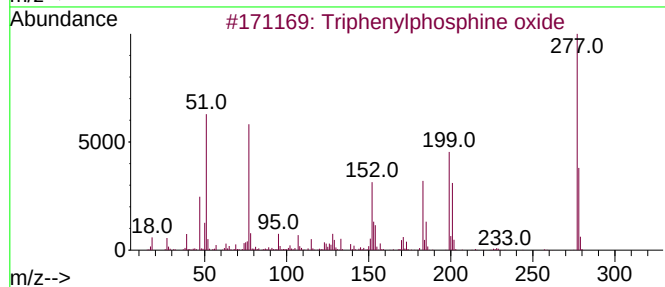
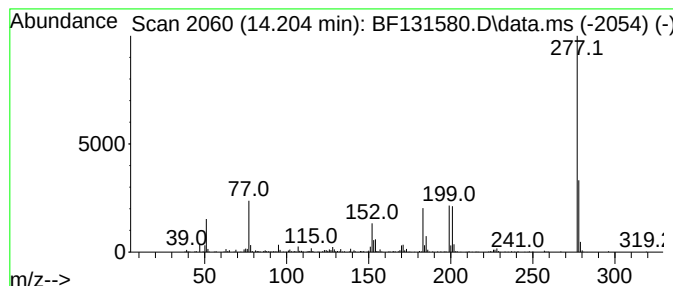
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Triphenylphosphine oxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.204	16.94 ng	326601	Chrysene-d12	14.104

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	92
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	58
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50
4			2-Phenyl-6-(trifluoromethyl)-1H-...	277	C15H10F3NO	1000387-59-3	32
5			5-quinolinol, 8-[2-(3,5-dimethyl...	277	C17H15N3O	1000397-10-2	9



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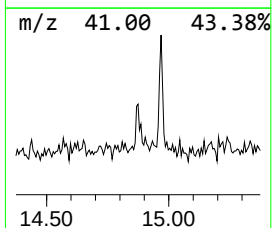
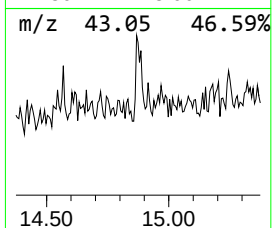
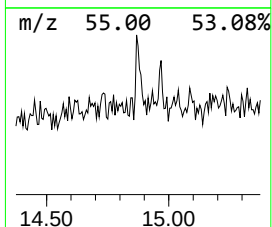
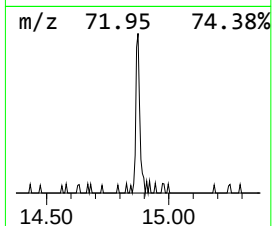
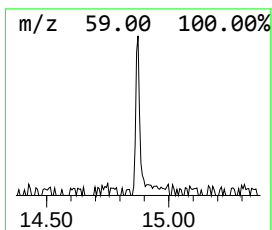
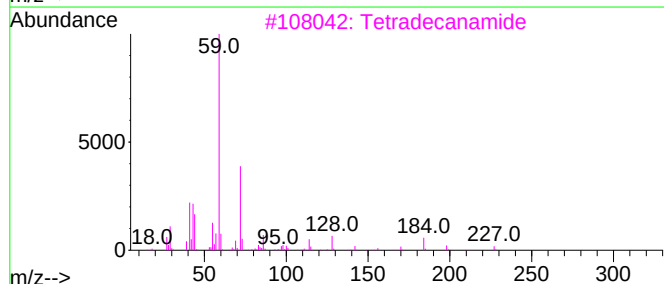
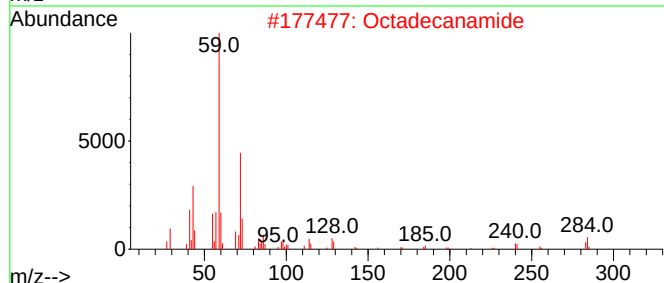
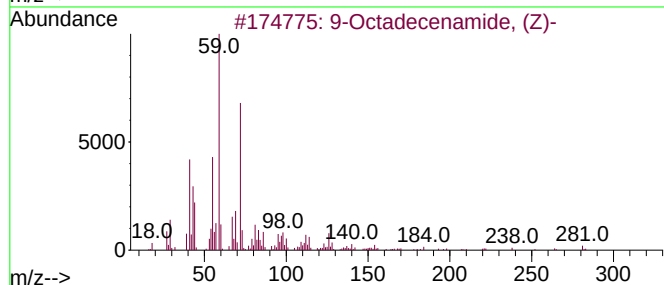
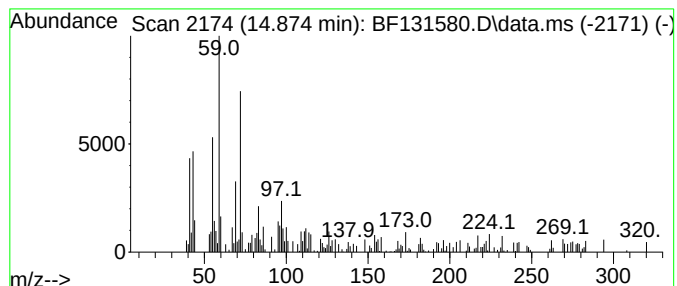
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.874	2.67 ng	46740	Perylene-d12	15.621	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
2	Octadecanamide	283	C18H37NO	000124-26-5	49
3	Tetradecanamide	227	C14H29NO	000638-58-4	43
4	Octanamide, N-propyl-N-isobutyl-	241	C15H31NO	1000437-67-3	42
5	Acetamide, N-propyl-N-(3-methylb...	171	C10H21NO	1010438-05-0	30



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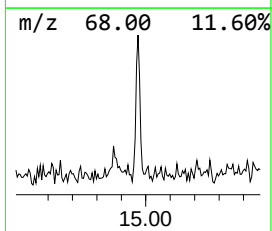
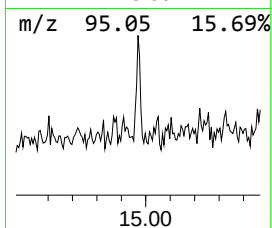
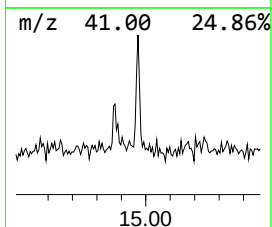
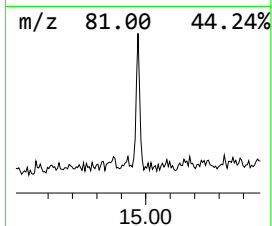
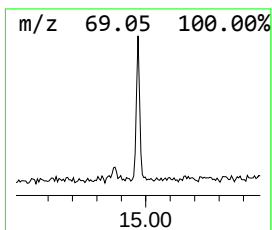
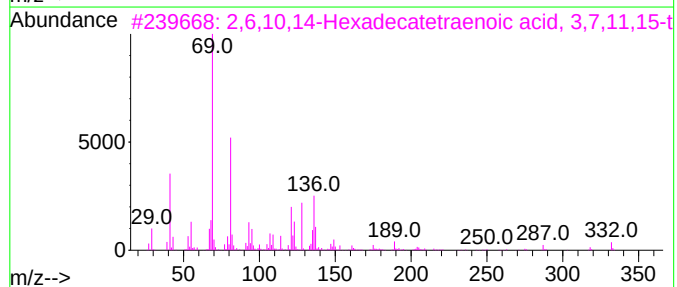
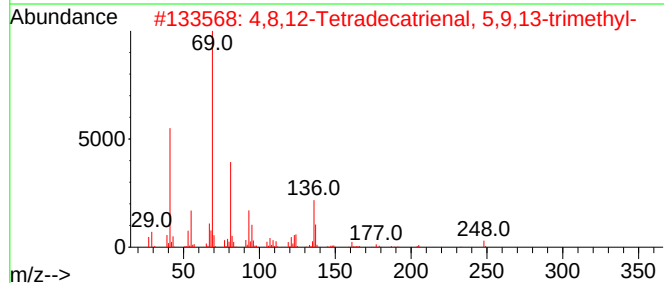
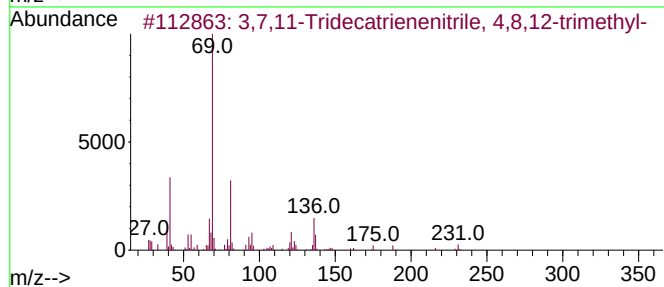
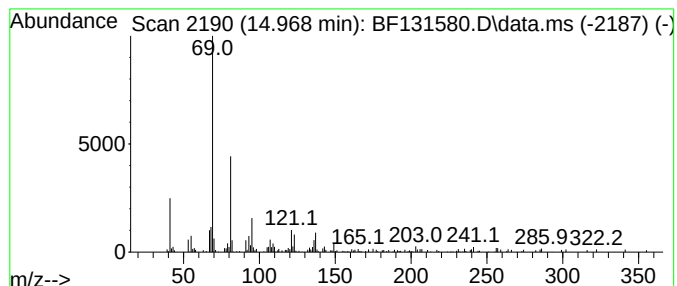
Instrument :
BNA_F
ClientSampleId :
TP-P

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 3,7,11-Tridecatrienitrile... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.968	4.06 ng	71182	Perylene-d12		15.621	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	3,7,11-Tridecatrienenitrile, 4,8...		231	C16H25N	006006-01-5	72
2	4,8,12-Tetradecatrienal, 5,9,13-...		248	C17H28O	066408-55-7	64
3	2,6,10,14-Hexadecatetraenoic aci...		332	C22H36O2	024035-35-6	64
4	Supraene		410	C30H50	007683-64-9	64
5	2,6-Octadiene, 4-methyl-		124	C9H16	074498-94-5	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120922\
Data File : BF131580.D
Acq On : 09 Dec 2022 22:25
Operator : CG\JU
Sample : N5965-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-P

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.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...	2.199	20.8	ng	429463	1	6.910	414034	20.0
2-Pentanone, 4-...	5.128	9.5	ng	196177	1	6.910	414034	20.0
Cyclohexane, 1,...	13.968	2.4	ng	45752	5	14.104	385585	20.0
Triphenylphosph...	14.204	16.9	ng	326601	5	14.104	385585	20.0
9-Octadecenamid...	14.874	2.7	ng	46740	6	15.621	350565	20.0
3,7,11-Tridecat...	14.968	4.1	ng	71182	6	15.621	350565	20.0