

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120922\
 Data File : BF131579.D
 Acq On : 09 Dec 2022 21:53
 Operator : CG\JU
 Sample : N5963-04
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RBR200046-03

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: BF131579.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.216	15	22	28	rBV	393929	497370	27.64%	3.941%
2	2.328	37	41	46	rBV	17744	22761	1.26%	0.180%
3	5.128	513	517	524	rVB	178764	201691	11.21%	1.598%
4	5.528	580	585	588	rBV	1569437	1440787	80.06%	11.416%
5	6.540	751	757	760	rBV	1524066	1487867	82.68%	11.789%
6	6.910	816	820	823	rBB	488605	421069	23.40%	3.336%
7	7.475	911	916	919	rBV	1041703	944562	52.49%	7.484%
8	8.198	1034	1039	1042	rBV	635077	524492	29.15%	4.156%
9	9.281	1217	1223	1226	rBV	2027566	1799575	100.00%	14.259%
10	9.963	1335	1339	1342	rVB	705356	617194	34.30%	4.890%
11	10.751	1469	1473	1476	rBV	1293631	1055056	58.63%	8.359%
12	11.451	1589	1592	1596	rBV	674460	607256	33.74%	4.811%
13	11.974	1673	1681	1685	rBV3	39669	44380	2.47%	0.352%
14	12.016	1685	1688	1690	rVB	23247	20511	1.14%	0.163%
15	12.674	1797	1800	1807	rVB2	16441	21655	1.20%	0.172%
16	12.898	1834	1838	1842	rVB	20143	20422	1.13%	0.162%
17	13.045	1859	1863	1866	rBV	1804101	1527170	84.86%	12.100%
18	13.957	2013	2018	2031	rBV4	49890	139381	7.75%	1.104%
19	14.080	2035	2039	2040	rBV	35324	34078	1.89%	0.270%
20	14.104	2040	2043	2047	rVB	454119	370919	20.61%	2.939%
21	14.204	2054	2060	2066	rBV	275732	326371	18.14%	2.586%
22	14.968	2186	2190	2195	rBV	98790	105287	5.85%	0.834%
23	15.168	2219	2224	2228	rBV3	12305	21719	1.21%	0.172%
24	15.615	2295	2300	2310	rVB	268174	342295	19.02%	2.712%
25	16.098	2378	2382	2387	rVB	18408	27183	1.51%	0.215%

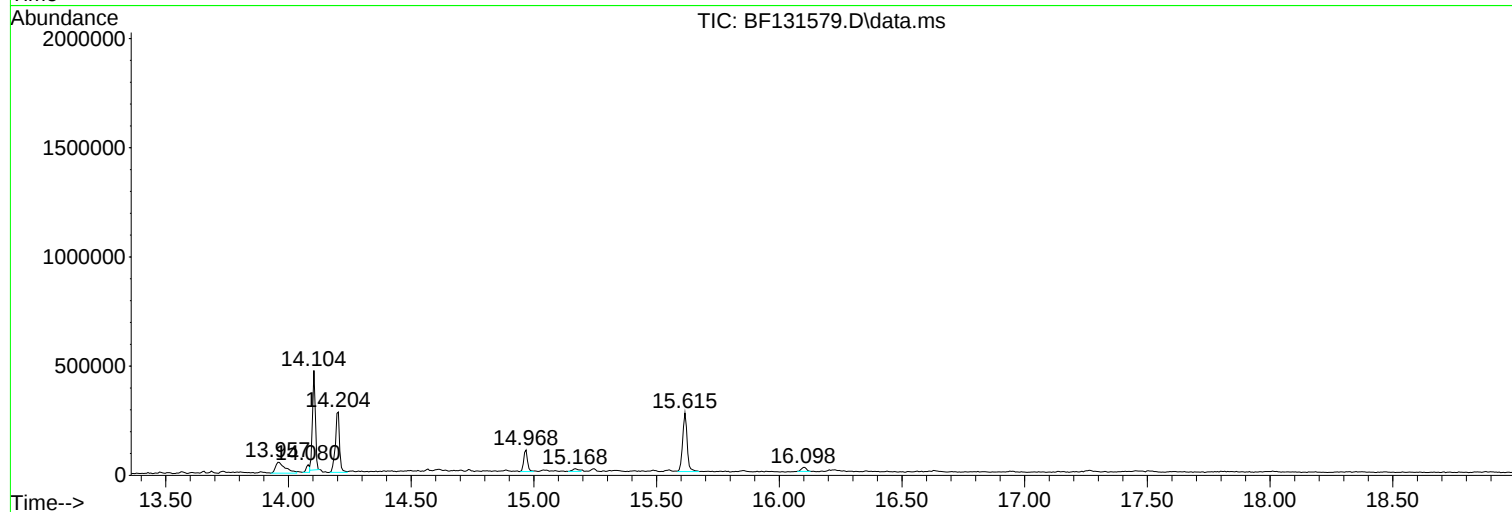
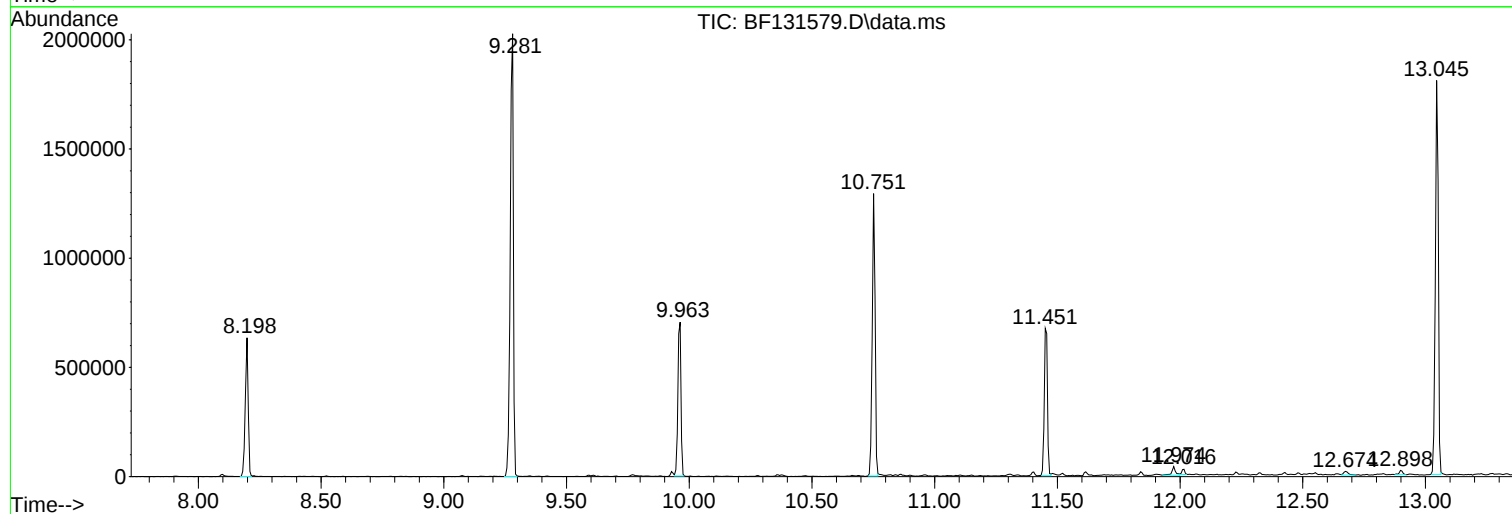
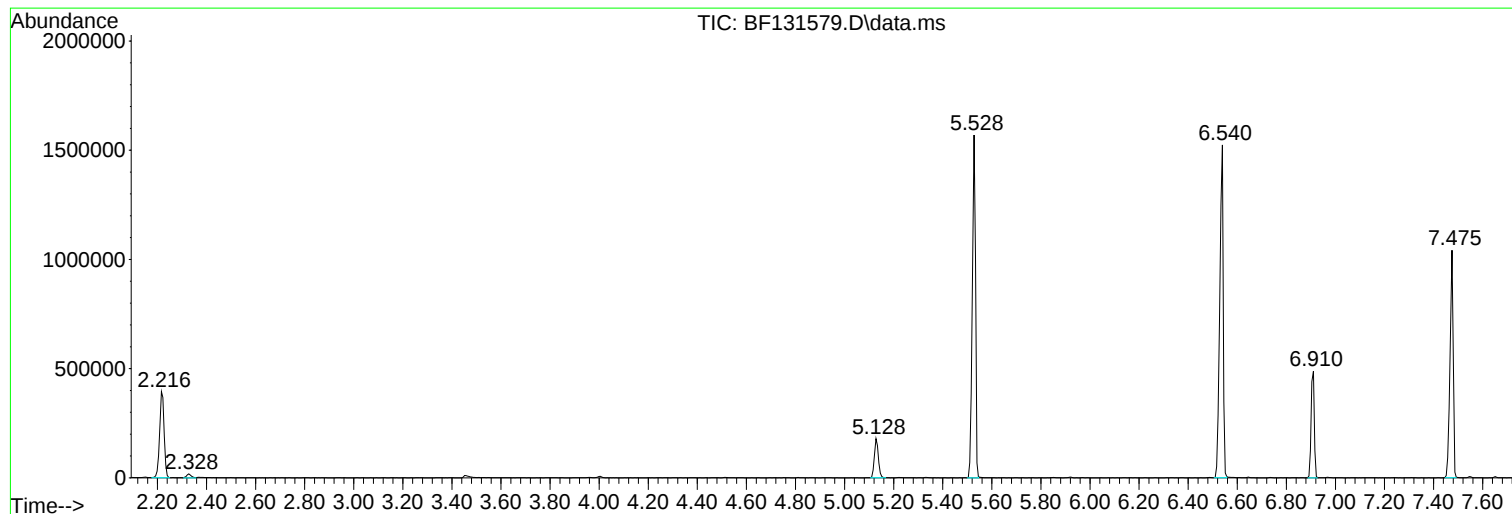
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ClientSampleId :
RBR200046-03

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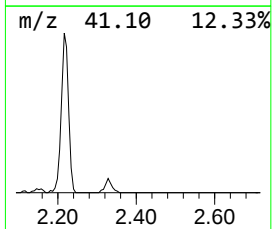
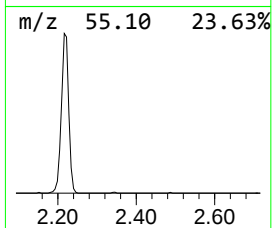
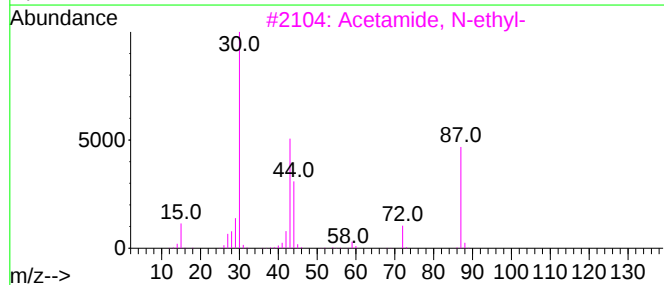
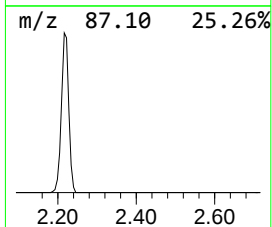
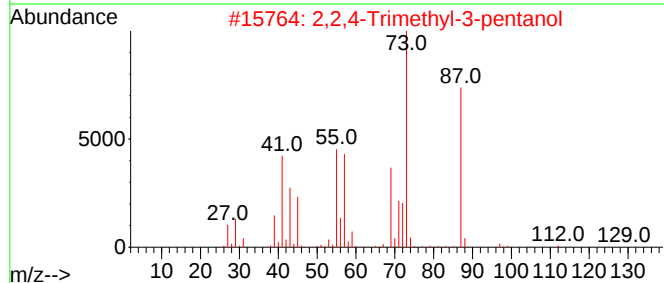
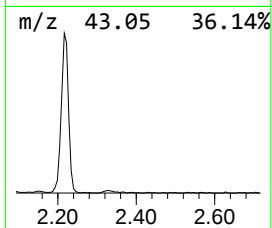
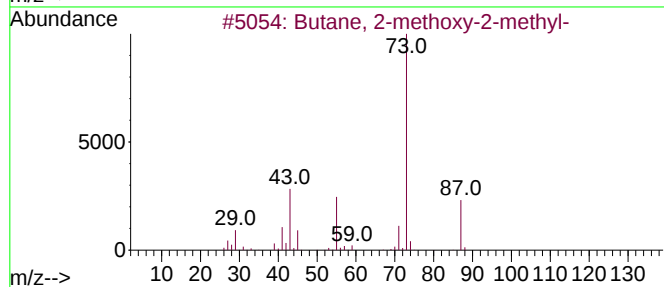
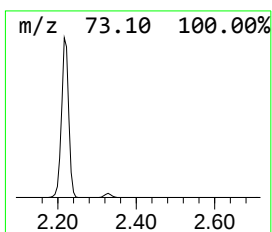
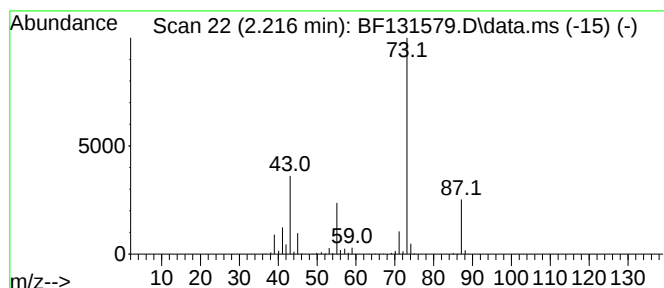
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.216	23.62 ng	497370	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	40
3			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
4			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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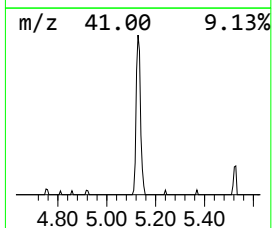
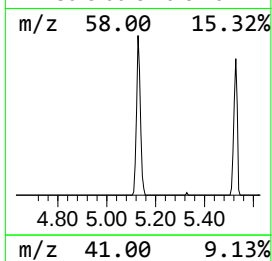
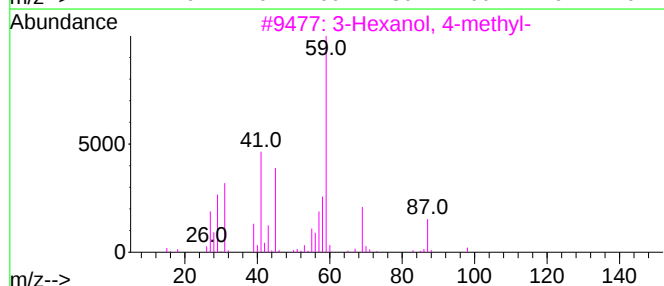
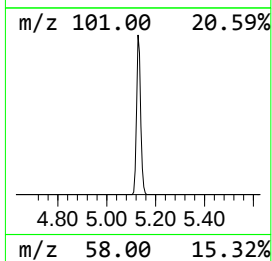
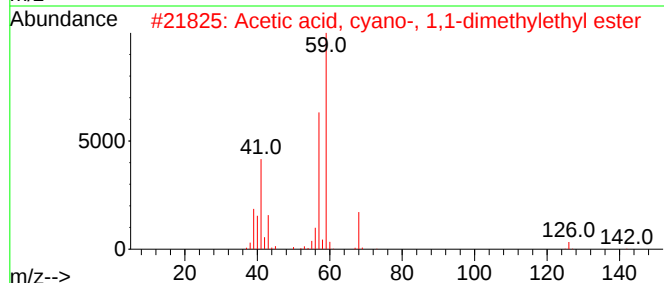
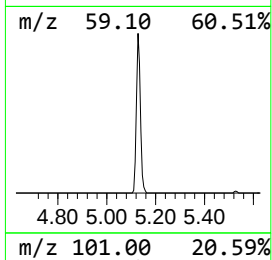
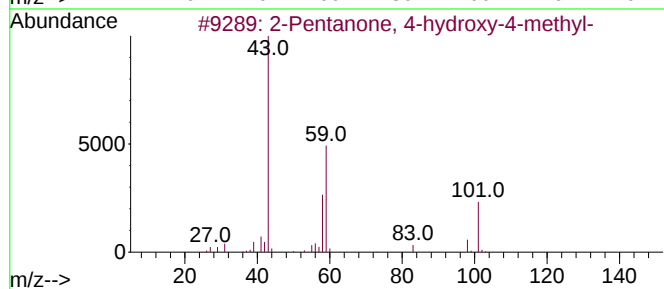
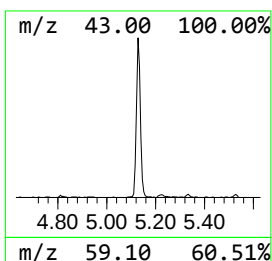
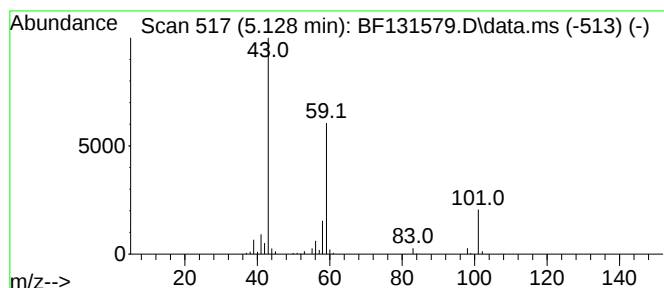
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.128	9.58 ng	201691	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	56
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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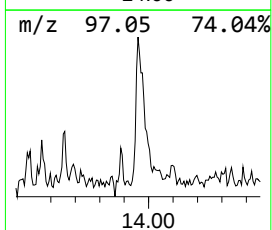
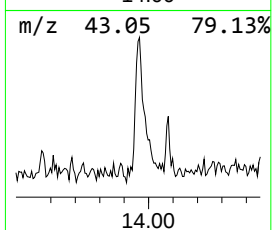
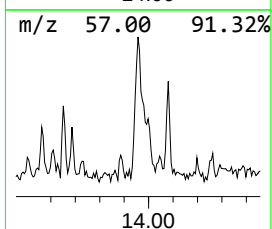
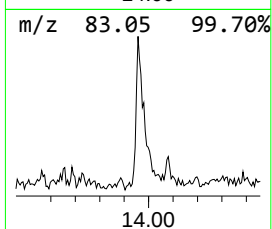
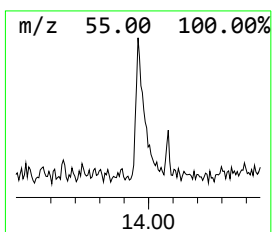
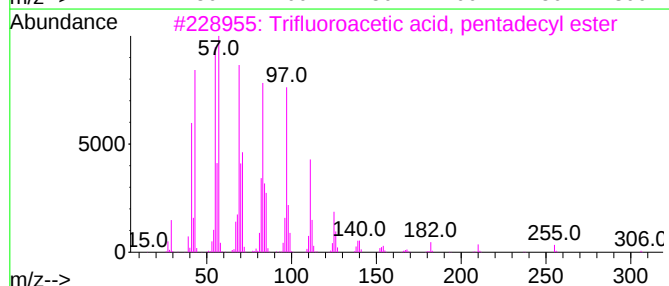
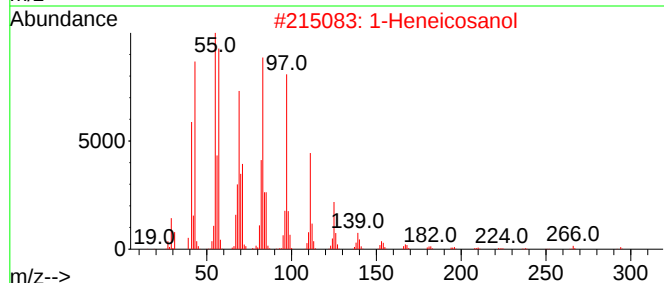
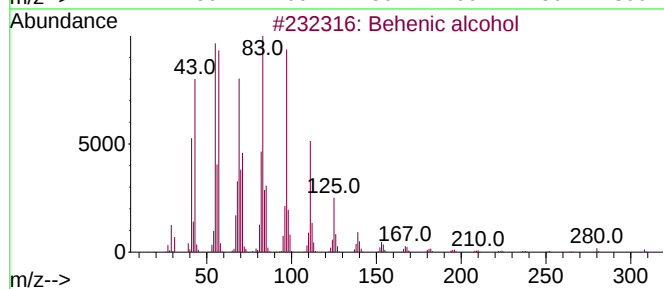
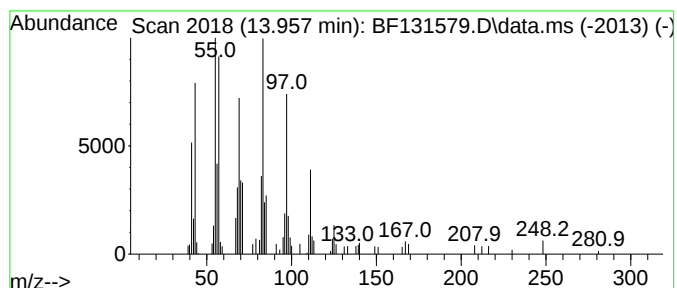
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Behenic alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.957	7.52 ng	139381	Chrysene-d12	14.104

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Behenic alcohol	326	C22H46O	000661-19-8	93
2			1-Heneicosanol	312	C21H44O	015594-90-8	90
3			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	81
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	81
5			n-Nonadecanol-1	284	C19H40O	001454-84-8	76



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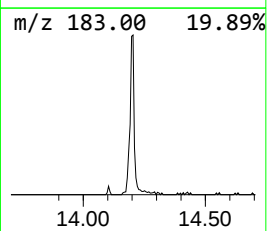
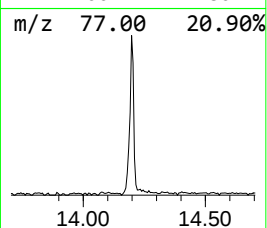
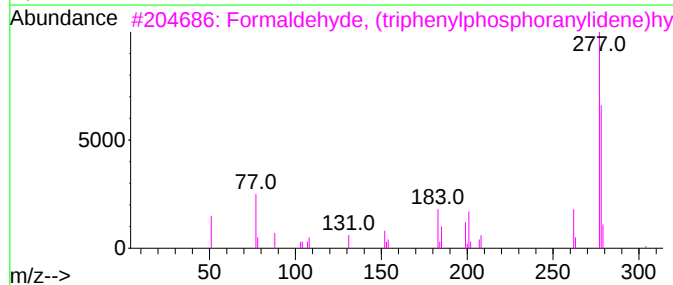
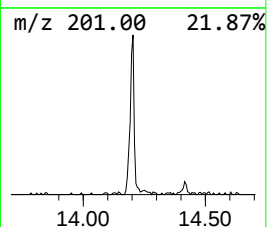
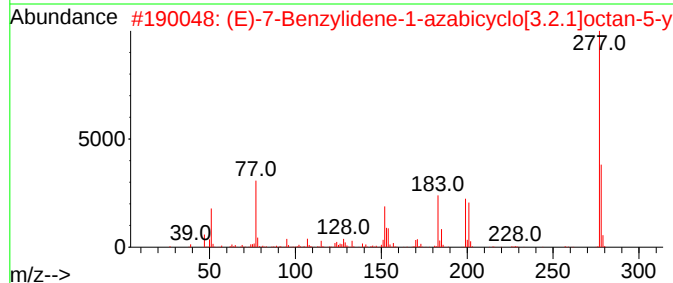
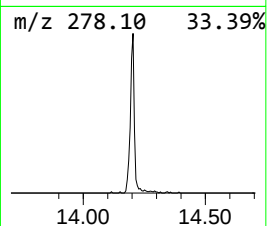
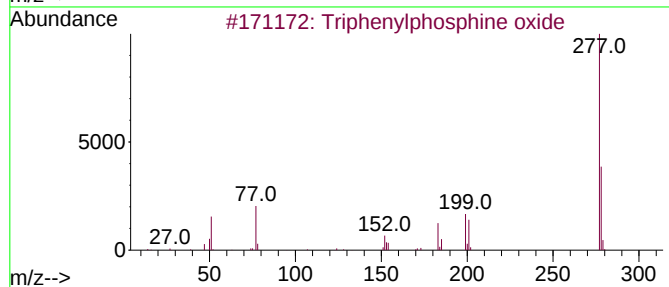
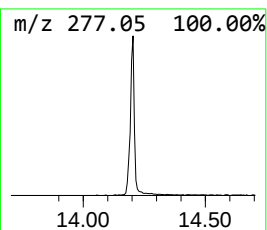
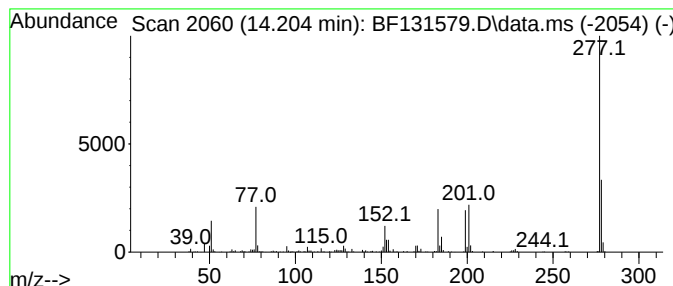
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Triphenylphosphine oxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.204	17.60 ng	326371	Chrysene-d12	14.104

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	93
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	76
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	42
4			2-Phenyl-6-(trifluoromethyl)-1H-...	277	C15H10F3NO	1000387-59-3	32
5			1H-Indole-3-acetic acid, 5-[(tri...	277	C14H19N03Si	072101-35-0	17



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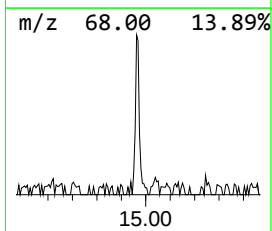
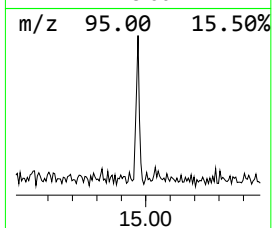
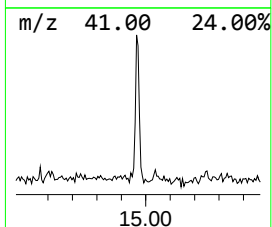
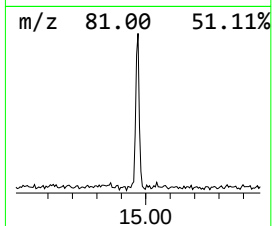
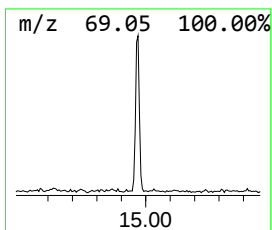
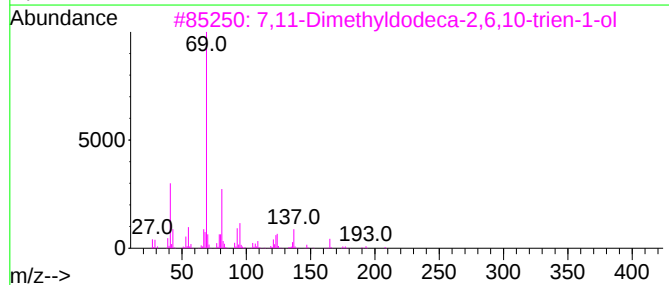
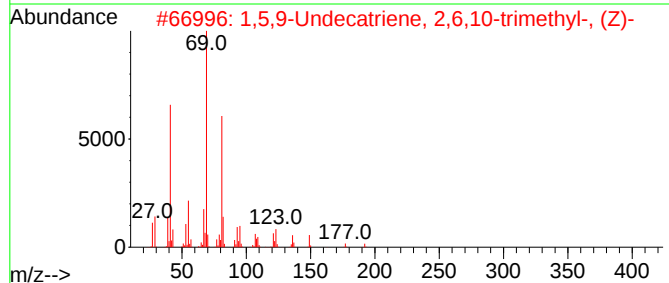
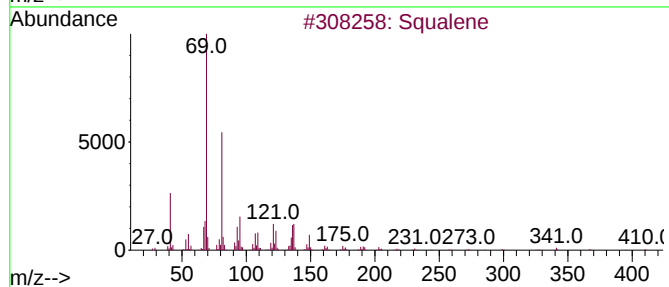
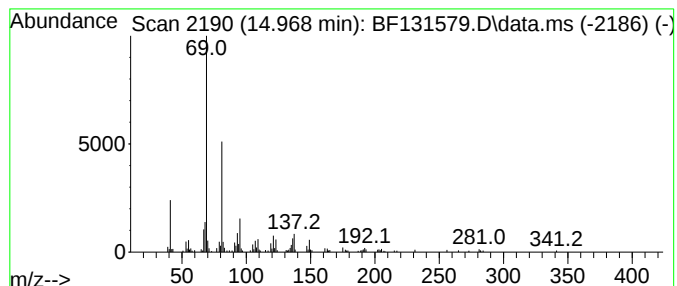
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.968	6.15 ng	105287	Perylene-d12	15.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	86
2			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	80
3			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
4			6,10,14-Hexadecatrien-1-ol, 3,7,...	292	C20H36O	036237-66-8	72
5			1,5-Heptadiene, 3,3,5-trimethyl-	138	C10H18	074630-29-8	59



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.216	23.6	ng	497370	1	6.910	421069	20.0
2-Pentanone, 4-...	5.128	9.6	ng	201691	1	6.910	421069	20.0
Behenic alcohol	13.957	7.5	ng	139381	5	14.104	370919	20.0
Triphenylphosph...	14.204	17.6	ng	326371	5	14.104	370919	20.0
Squalene	14.968	6.2	ng	105287	6	15.615	342295	20.0