

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102723\
 Data File : BF135983.D
 Acq On : 27 Oct 2023 14:25
 Operator : CG\JU
 Sample : 04767-04
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EB-1

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-BF102523.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135983.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	18	22	28	rVB	58658	74856	1.48%	0.241%
2	5.045	500	503	511	rVB	218732	257728	5.11%	0.831%
3	5.451	567	572	575	rBV	2474175	2247154	44.56%	7.249%
4	6.445	726	741	747	rBV2	1590831	1756948	34.84%	5.668%
5	6.581	760	764	769	rBV2	71031	63072	1.25%	0.203%
6	6.822	802	805	809	rBV	1119421	951661	18.87%	3.070%
7	7.204	854	870	872	rBV	264548	614028	12.18%	1.981%
8	7.222	872	873	877	rVB	176957	136256	2.70%	0.440%
9	7.387	894	901	904	rBV	2839769	2905916	57.62%	9.374%
10	7.834	973	977	984	rBV	98793	103193	2.05%	0.333%
11	8.104	1019	1023	1026	rBV	1749591	1293794	25.66%	4.174%
12	8.328	1058	1061	1064	rBV	70182	72989	1.45%	0.235%
13	8.357	1064	1066	1076	rVB	100795	112698	2.23%	0.364%
14	8.445	1076	1081	1085	rBV3	94679	111910	2.22%	0.361%
15	9.186	1203	1207	1210	rBV	5985397	5042992	100.00%	16.268%
16	9.304	1224	1227	1232	rVB2	125110	172051	3.41%	0.555%
17	9.863	1318	1322	1325	rVB	1804138	1384473	27.45%	4.466%
18	10.069	1350	1357	1362	rBV2	105680	120937	2.40%	0.390%
19	10.410	1412	1415	1422	rVB	79772	62438	1.24%	0.201%
20	10.657	1452	1457	1460	rBV	3312301	3139956	62.26%	10.129%
21	11.157	1539	1542	1545	rVB	121203	106490	2.11%	0.344%
22	11.351	1572	1575	1578	rBV	1449969	1356349	26.90%	4.375%
23	11.374	1578	1579	1583	rVV	565229	371727	7.37%	1.199%
24	11.427	1585	1588	1591	rVB	119547	98735	1.96%	0.319%
25	11.580	1608	1614	1617	rBV	91394	91404	1.81%	0.295%
26	11.892	1663	1667	1671	rBV2	201631	211731	4.20%	0.683%
27	11.969	1677	1680	1682	rBV	63123	57128	1.13%	0.184%
28	12.569	1779	1782	1786	rBV	367558	325625	6.46%	1.050%
29	12.604	1786	1788	1796	rVB3	126043	170506	3.38%	0.550%
30	12.686	1796	1802	1805	rBV2	71816	84391	1.67%	0.272%
31	12.798	1815	1821	1828	rBV	247954	243258	4.82%	0.785%
32	12.957	1843	1848	1851	rBV	4296424	4038490	80.08%	13.028%
33	13.333	1908	1912	1927	rBV	894660	1268309	25.15%	4.091%
34	14.010	2022	2027	2030	rBV	849270	860500	17.06%	2.776%
35	14.110	2038	2044	2047	rBV	76229	89493	1.77%	0.289%
36	14.792	2156	2160	2163	rBV	48996	60792	1.21%	0.196%

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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

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102523.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.492	2274	2279	2287	rVB	731911	938932	18.62%	3.029%
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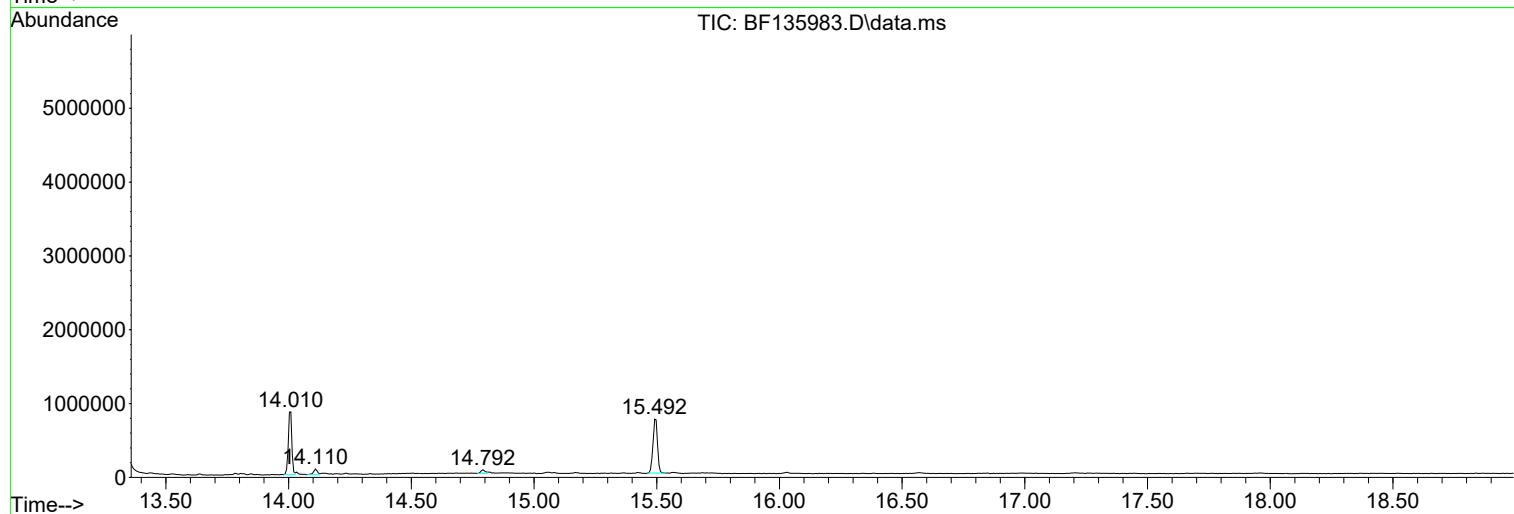
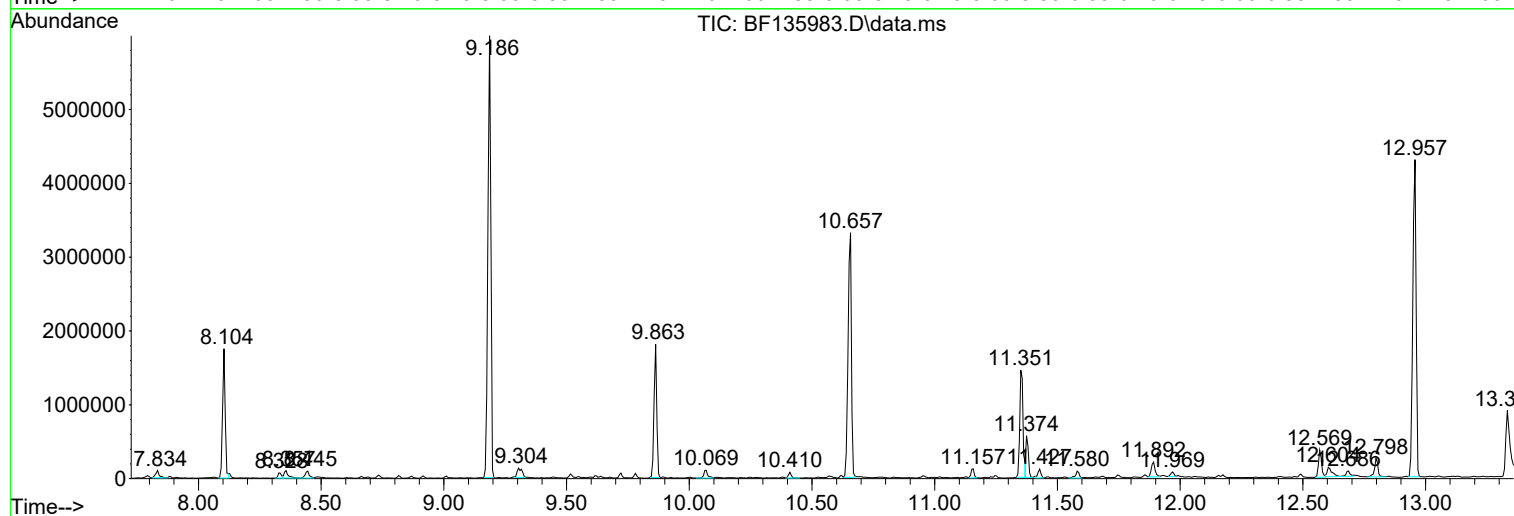
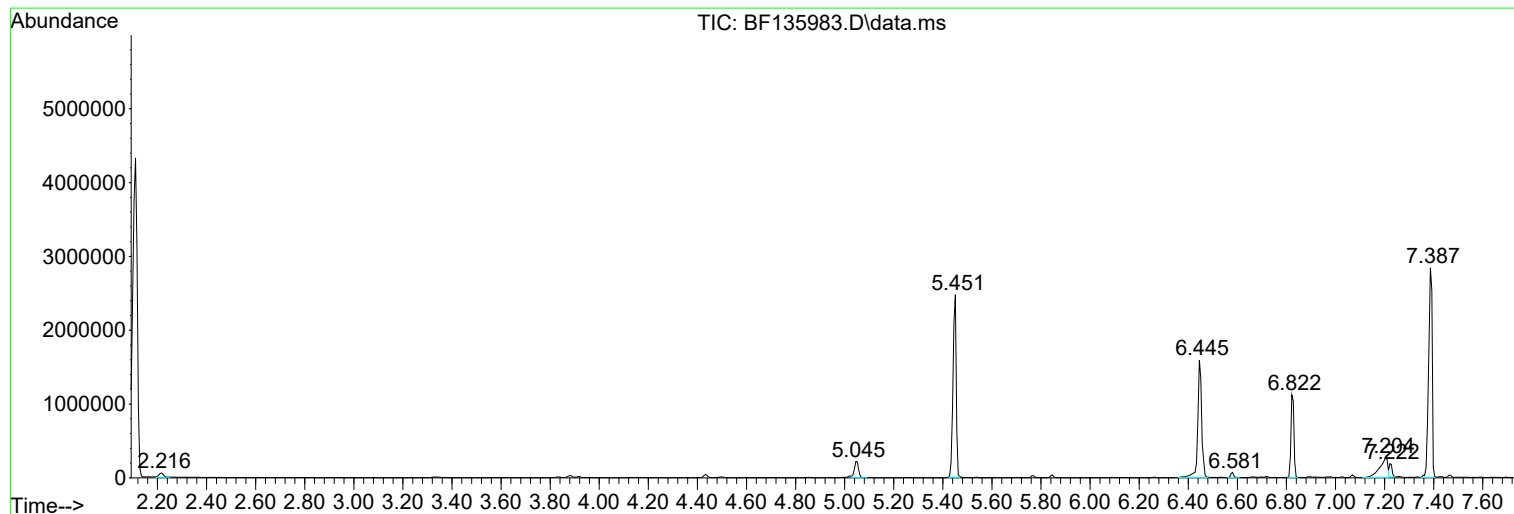
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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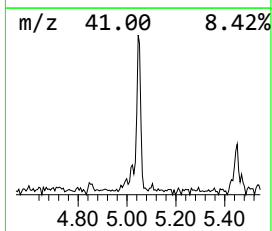
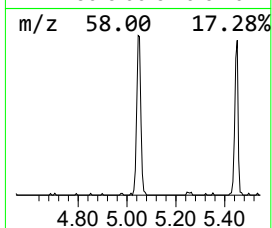
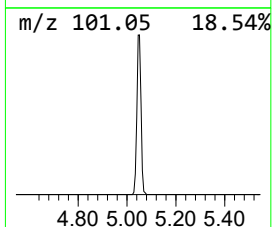
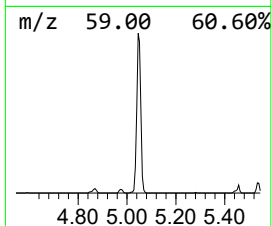
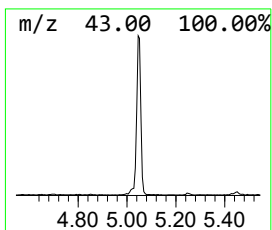
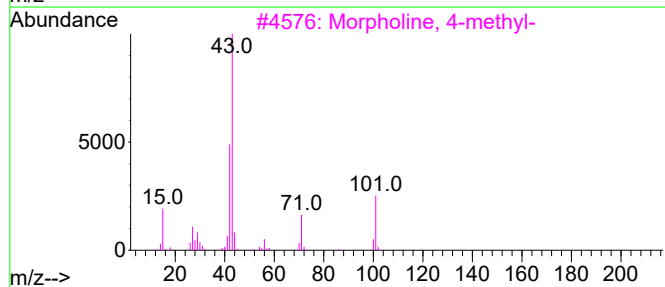
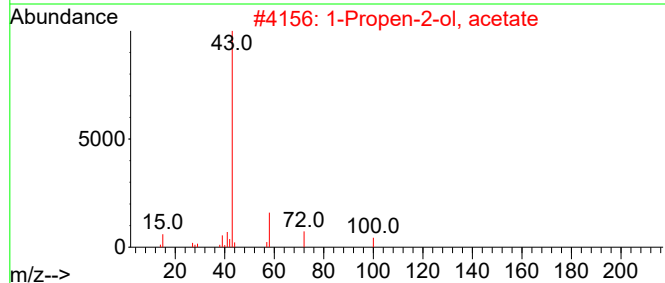
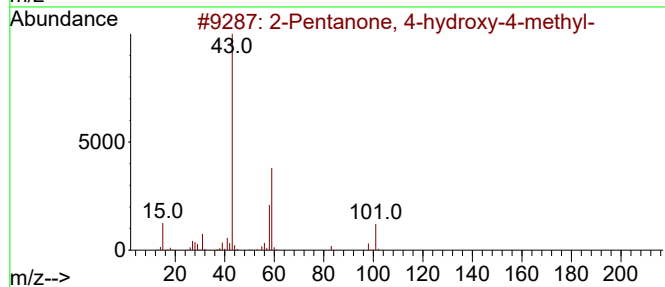
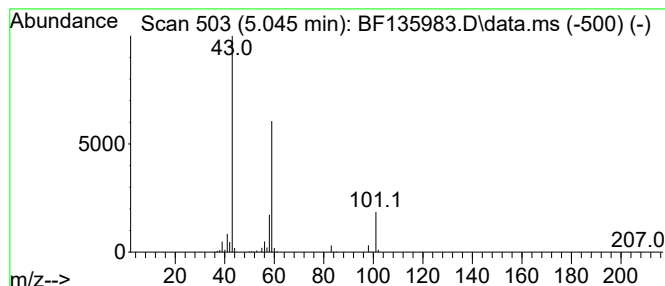
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.045	5.42 ng	257728	1,4-Dichlorobenzene-d4	6.828

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
3			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4			Acetone	58	C3H6O	000067-64-1	9
5			Allyl acetate	100	C5H8O2	000591-87-7	9



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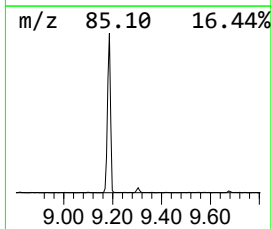
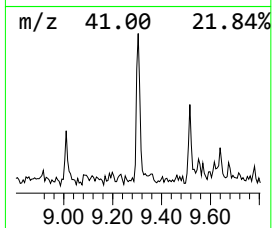
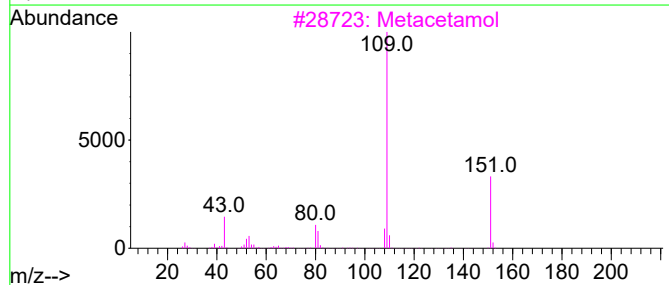
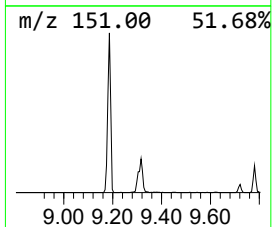
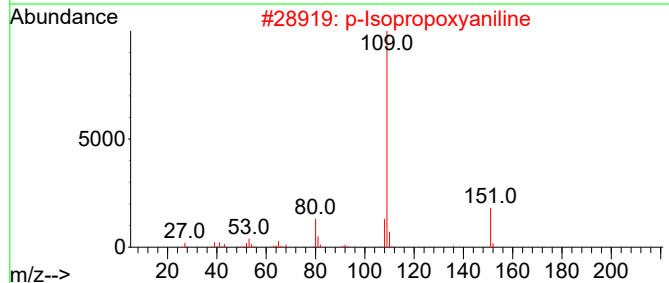
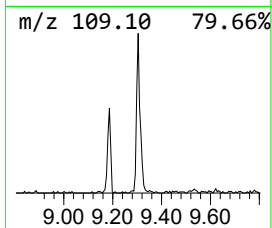
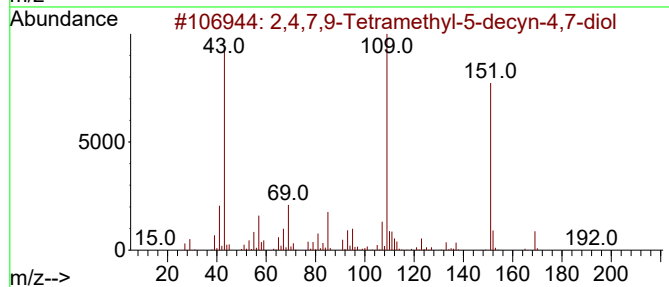
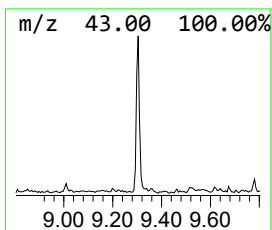
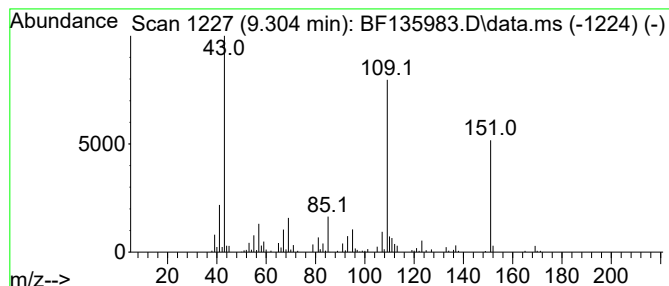
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.304	2.49 ng	172051	Acenaphthene-d10	9.863

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2		000126-86-3	91
2	p-Isopropoxyaniline	151	C9H13NO		007664-66-6	53
3	Metacetamol	151	C8H9NO2		000621-42-1	53
4	m-Isopropoxyaniline	151	C9H13NO		041406-00-2	53
5	Cyclohexanol, 3,3,5-trimethyl-	142	C9H18O		000116-02-9	47



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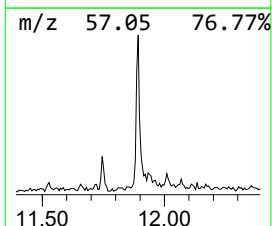
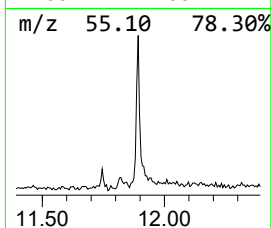
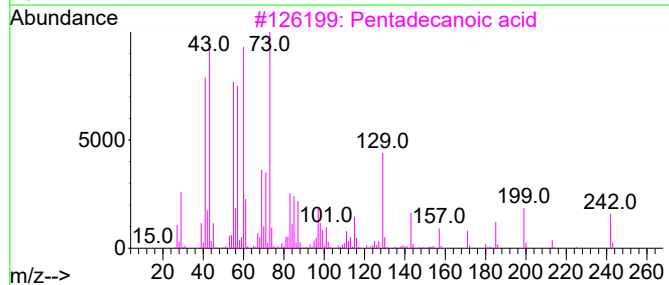
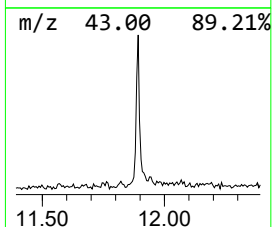
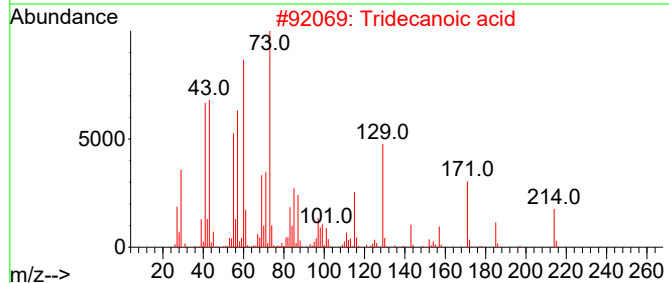
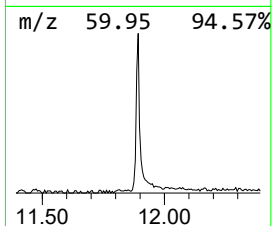
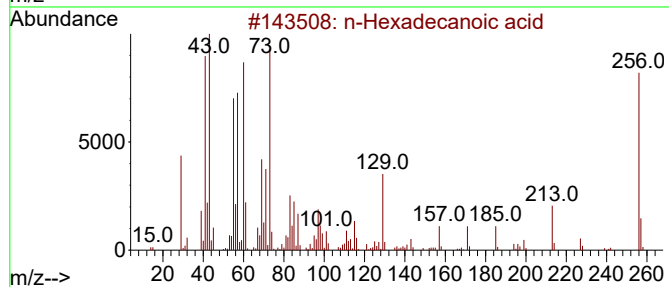
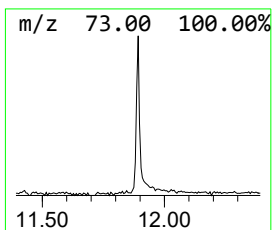
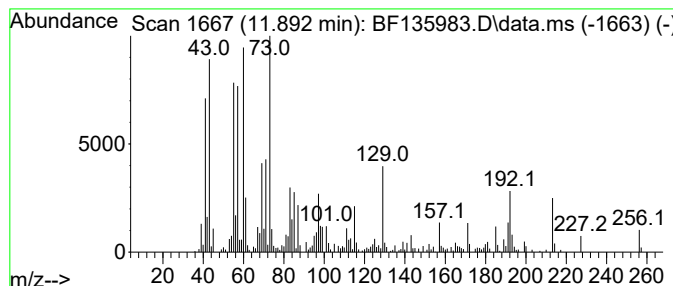
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.892	3.12 ng	211731	Phenanthrene-d10	11.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			Undecanoic acid	186	C11H22O2	000112-37-8	74
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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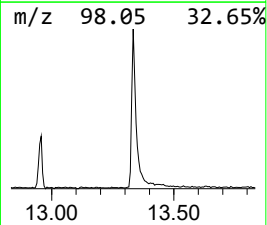
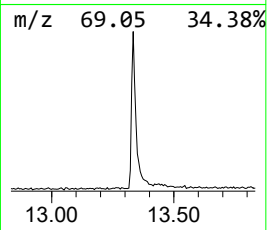
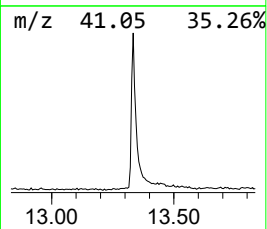
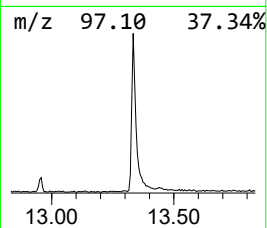
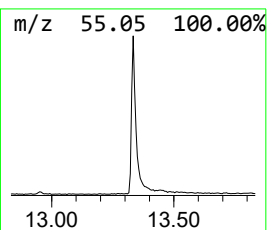
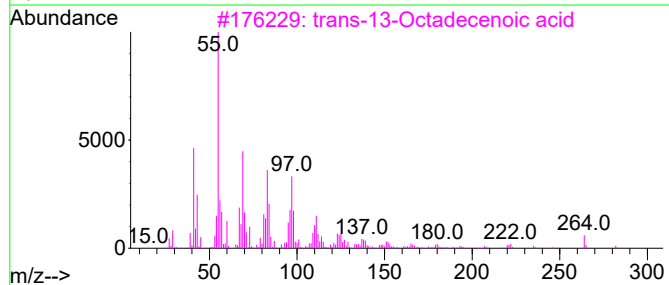
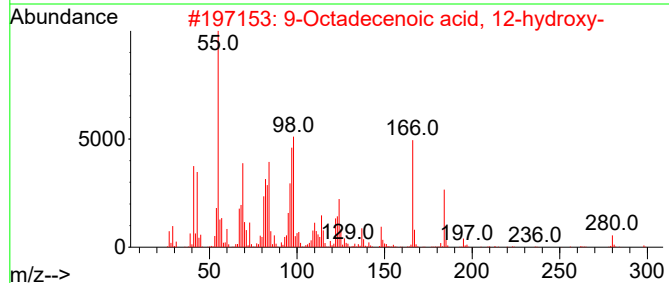
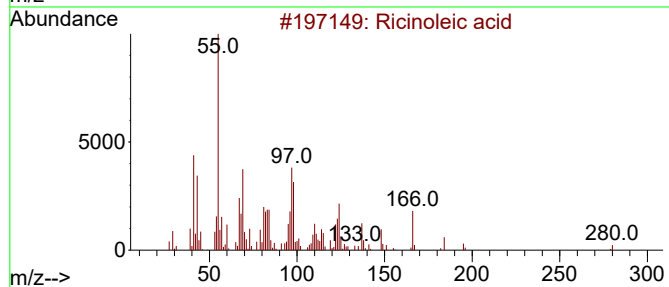
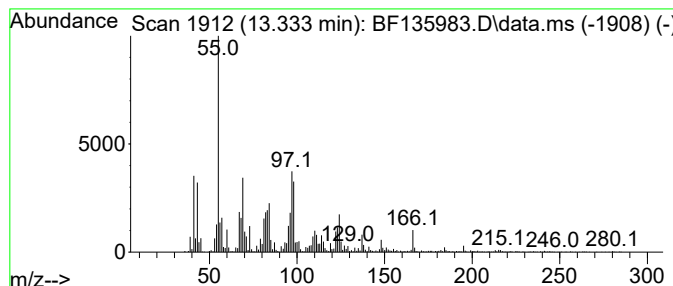
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Ricinoleic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.333	29.48 ng	1268310	Chrysene-d12	14.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ricinoleic acid	298	C18H34O3	000141-22-0	90
2			9-Octadecenoic acid, 12-hydroxy-	298	C18H34O3	007431-95-0	86
3			trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	53
4			9-Octadecenoic acid, 12-hydroxy-...	312	C19H36O3	000141-24-2	49
5			Ethyl 9-hexadecenoate	282	C18H34O2	054546-22-4	43



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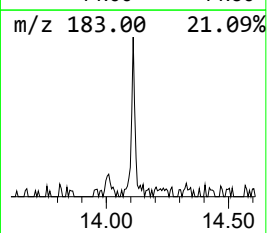
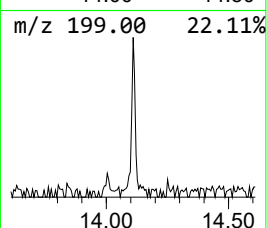
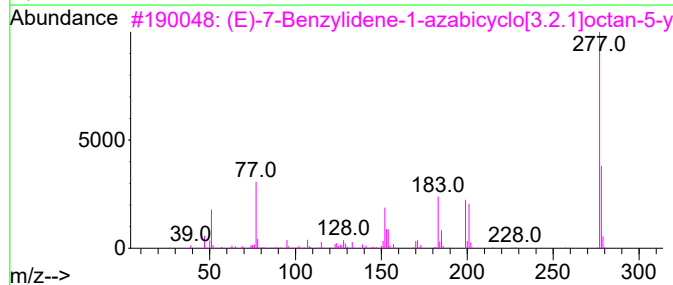
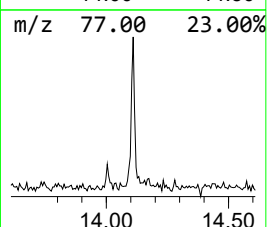
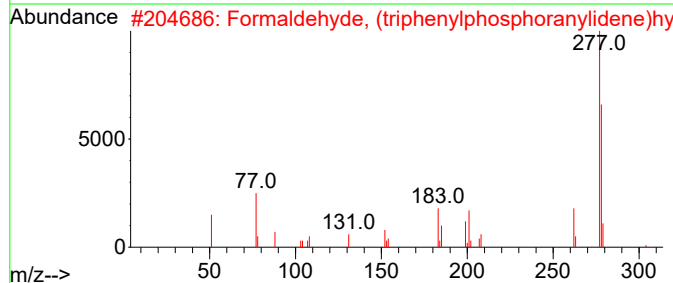
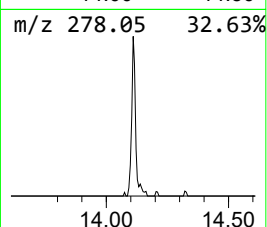
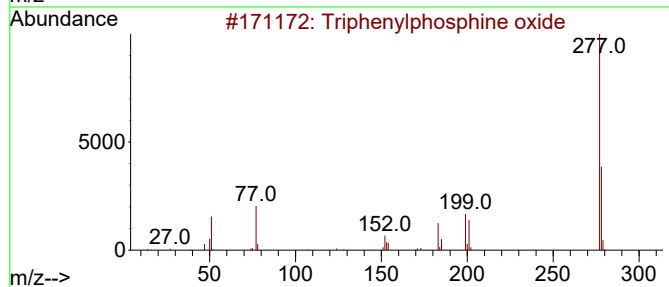
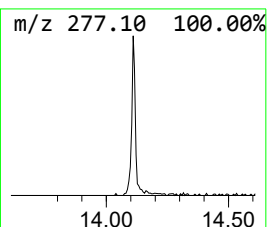
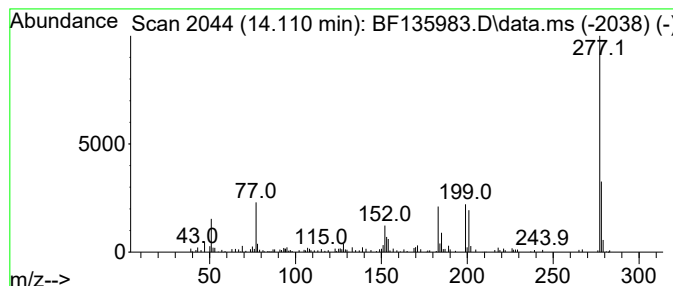
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Triphenylphosphine oxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.110	2.08 ng	89493	Chrysene-d12	14.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	94
2			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	64
3			(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19N03S	1000483-83-4	52
4			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	37
5			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	23



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102723\
Data File : BF135983.D
Acq On : 27 Oct 2023 14:25
Operator : CG\JU
Sample : 04767-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EB-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.045	5.4	ng	257728	1	6.828	951661	20.0
2,4,7,9-Tetrame...	9.304	2.5	ng	172051	3	9.863	1384470	20.0
n-Hexadecanoic ...	11.892	3.1	ng	211731	4	11.351	1356350	20.0
Ricinoleic acid	13.333	29.5	ng	1268310	5	14.010	860500	20.0
Triphenylphosph...	14.110	2.1	ng	89493	5	14.010	860500	20.0