

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112522\
 Data File : BF131392.D
 Acq On : 25 Nov 2022 12:54
 Operator : CG\JU
 Sample : N5742-09
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-45

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-BF112122.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131392.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.299	25	36	41	rVB	1716985	2403320	66.05%	10.446%
2	5.181	521	526	536	rVB	222776	256045	7.04%	1.113%
3	5.569	587	592	595	rVB	1806048	1631472	44.84%	7.091%
4	6.569	757	762	765	rBV	1238382	1232094	33.86%	5.355%
5	6.957	824	828	831	rVB	696448	598028	16.44%	2.599%
6	7.522	918	924	927	rBV	1974594	2082602	57.24%	9.052%
7	8.245	1042	1047	1050	rBV	929516	776496	21.34%	3.375%
8	9.328	1225	1231	1234	rBV	4049684	3638609	100.00%	15.815%
9	10.010	1342	1347	1350	rBV	1092338	891669	24.51%	3.876%
10	10.804	1477	1482	1485	rBV	2181088	1905340	52.36%	8.281%
11	11.504	1597	1601	1605	rBV	936492	858379	23.59%	3.731%
12	12.033	1683	1691	1705	rBV	740089	901875	24.79%	3.920%
13	12.827	1818	1826	1847	rVB	1292465	1650147	45.35%	7.172%
14	12.998	1852	1855	1863	rVB3	33005	49685	1.37%	0.216%
15	13.104	1868	1873	1877	rBV	2883139	2916309	80.15%	12.675%
16	14.163	2050	2053	2057	rVB	625138	526273	14.46%	2.287%
17	14.257	2066	2069	2076	rVB	73303	79887	2.20%	0.347%
18	15.045	2199	2203	2208	rVB	63550	69498	1.91%	0.302%
19	15.704	2309	2315	2319	rBV2	424032	539831	14.84%	2.346%

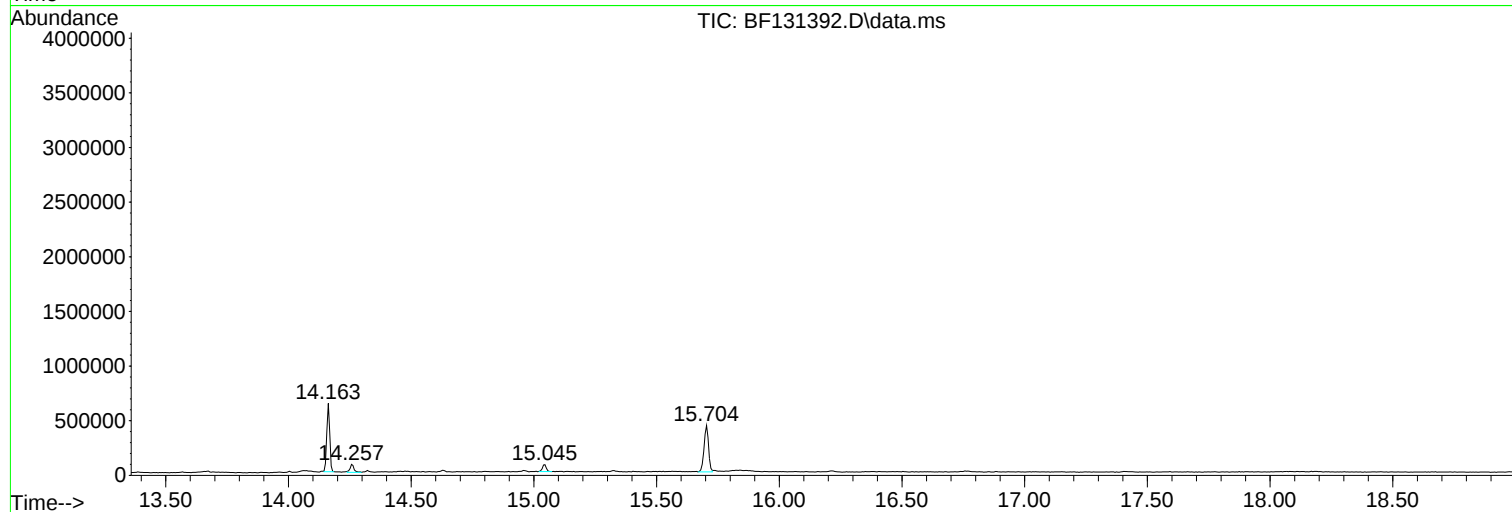
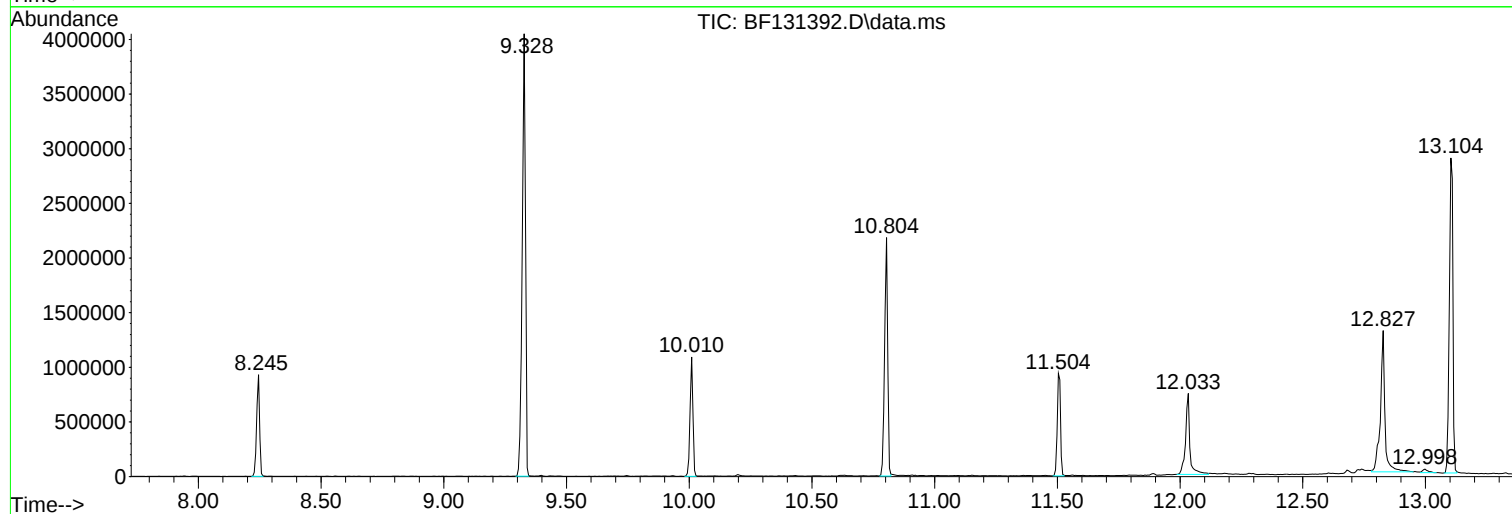
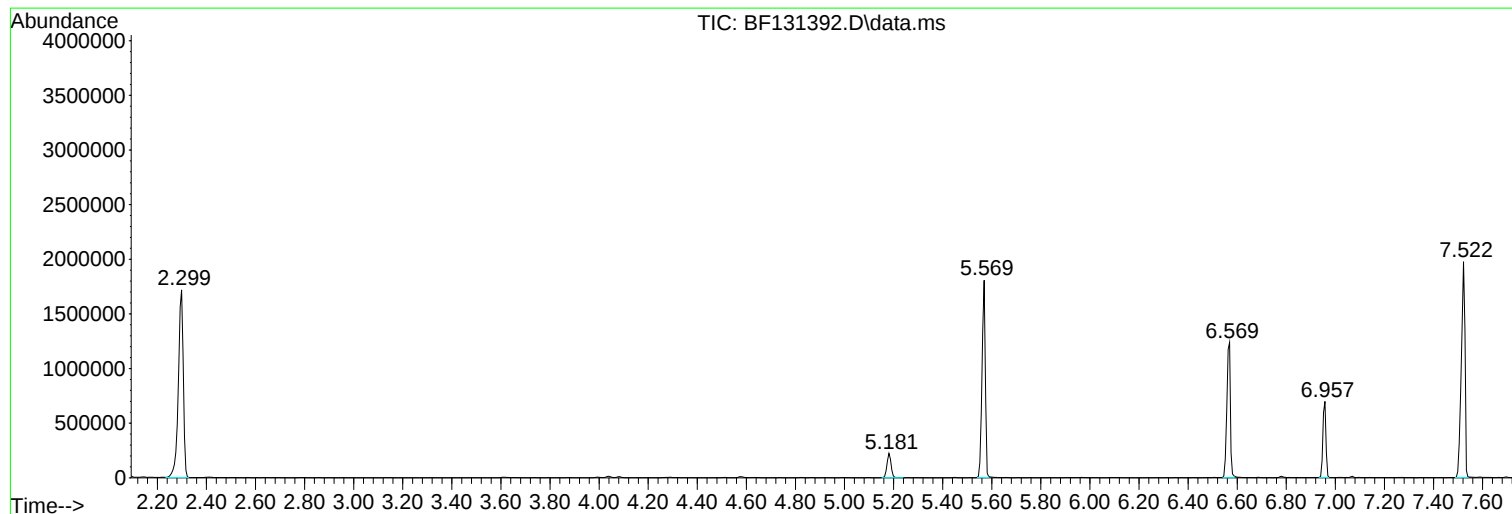
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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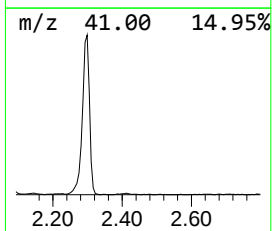
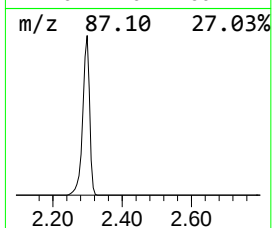
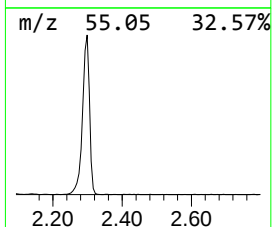
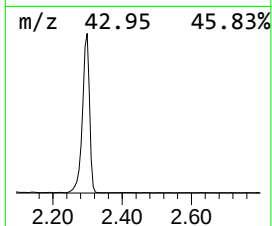
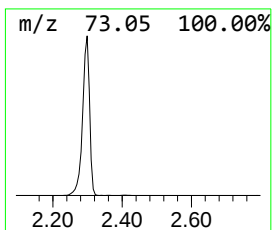
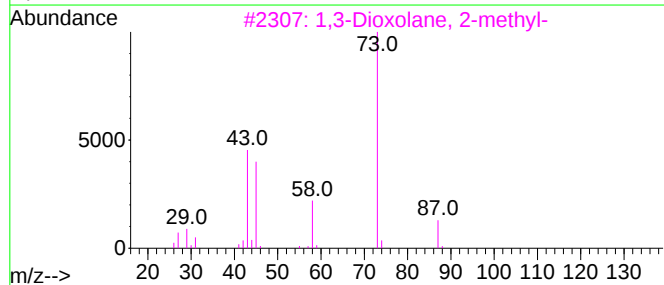
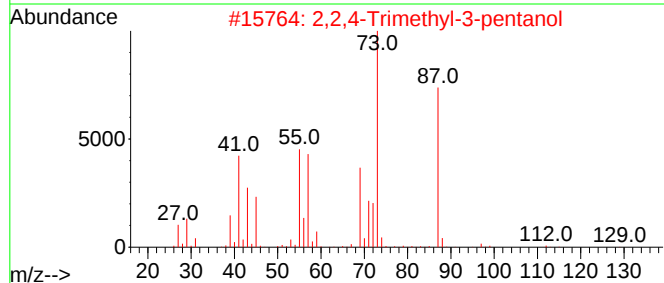
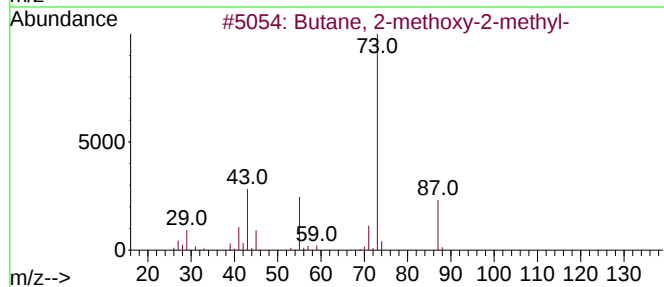
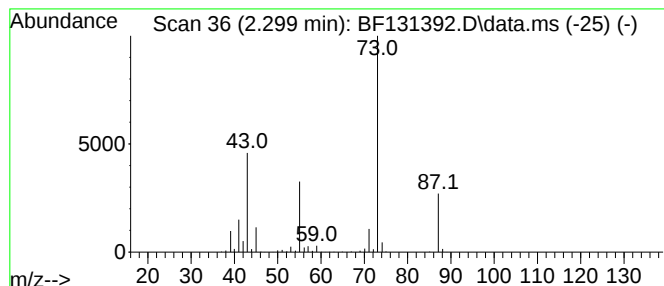
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.299	80.37 ng	2403320	1,4-Dichlorobenzene-d4	6.957

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			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	12



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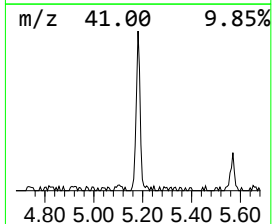
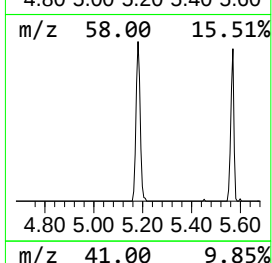
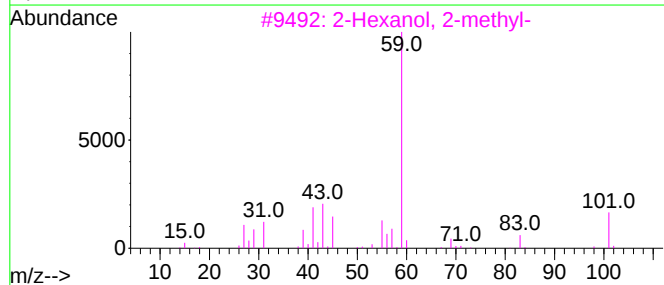
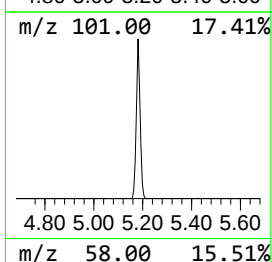
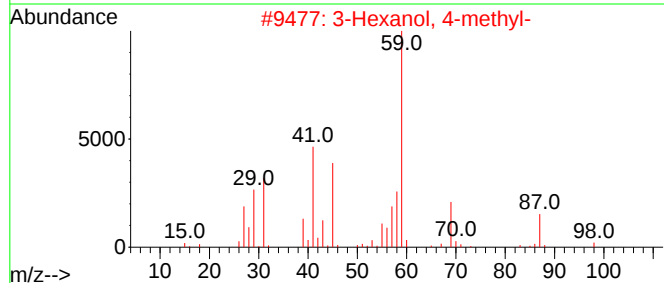
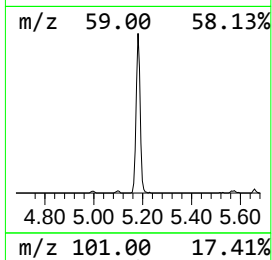
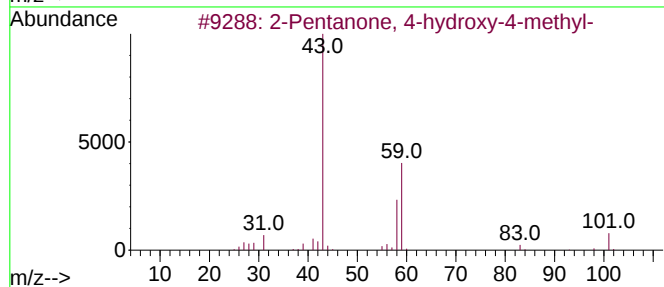
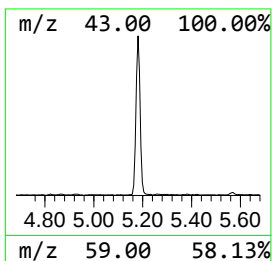
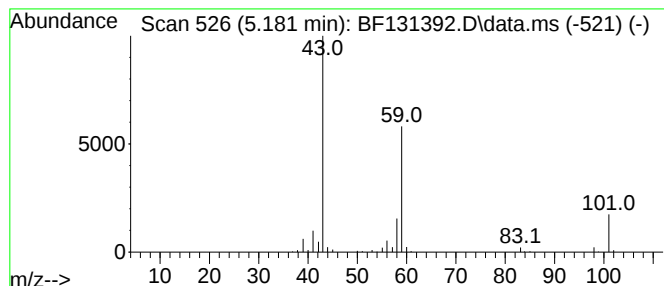
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.181	8.56 ng	256045	1,4-Dichlorobenzene-d4	6.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12



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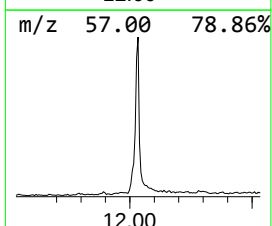
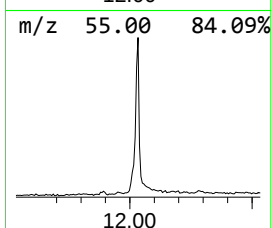
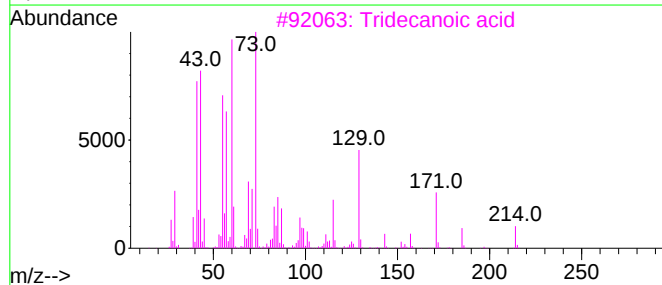
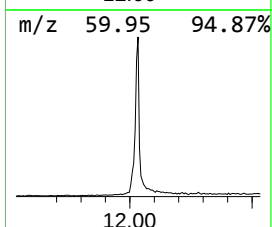
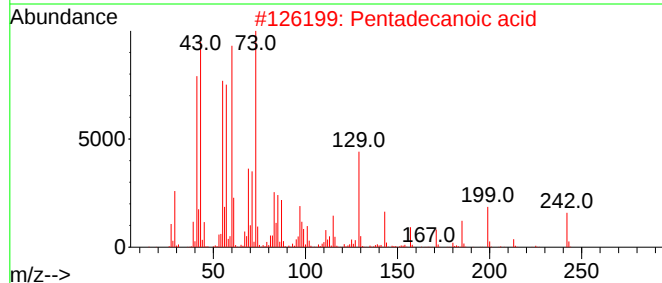
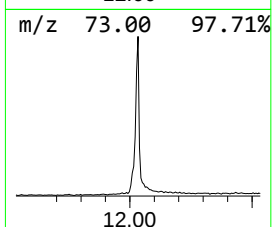
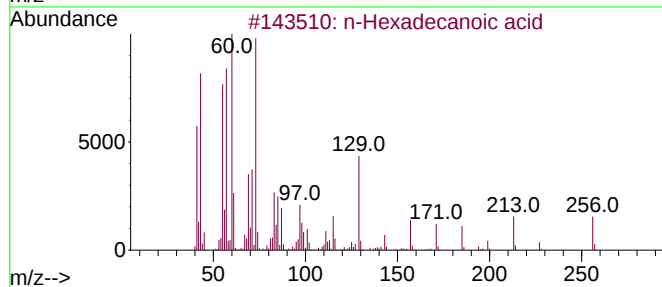
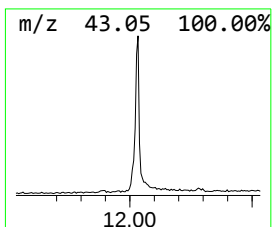
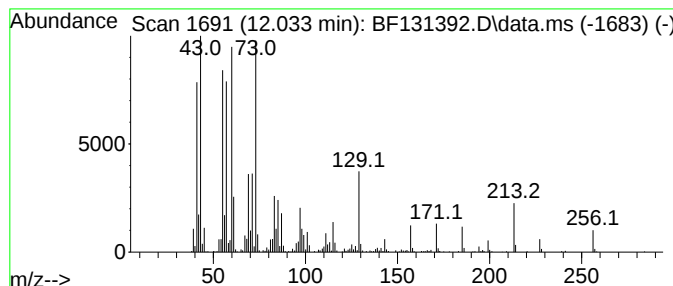
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.033	21.01 ng	901875	Phenanthrene-d10	11.504

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Tridecanoic acid	214	C13H26O2	000638-53-9	89
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			Undecanoic acid	186	C11H22O2	000112-37-8	58



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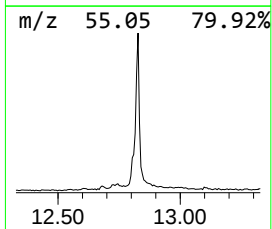
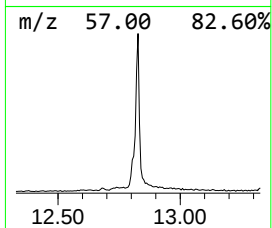
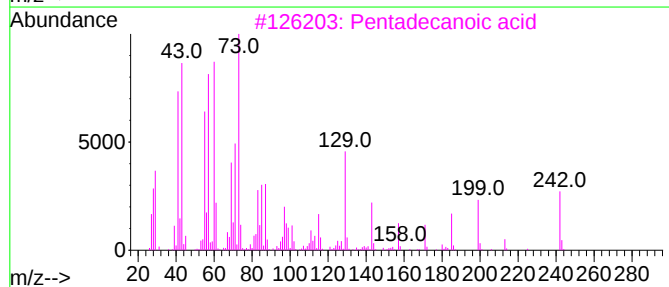
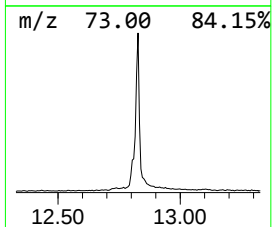
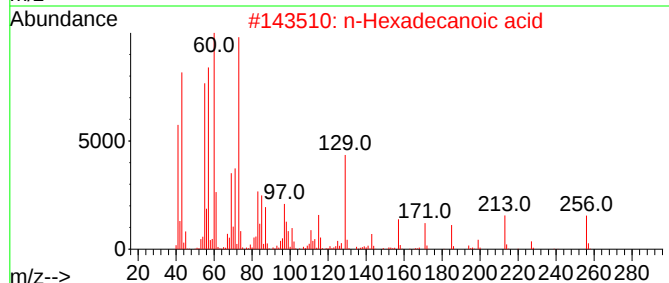
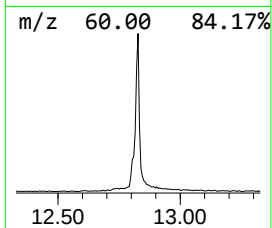
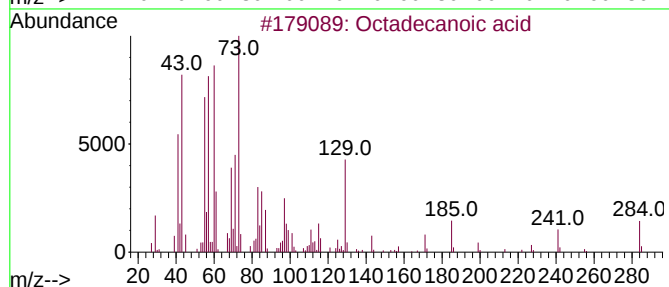
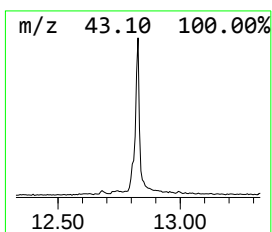
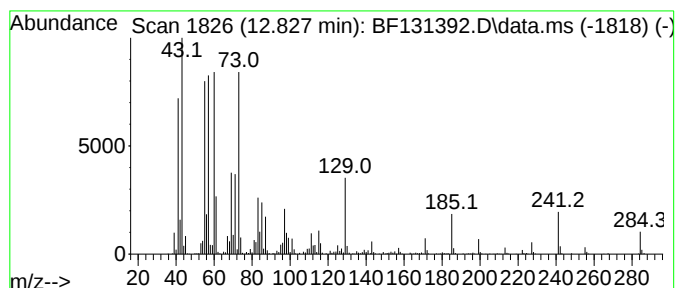
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Peak Number 4 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.827	38.45 ng	1650150	Phenanthrene-d10		11.504	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Octadecanoic acid		284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	93
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	89
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	62
5	Undecanoic acid		186	C11H22O2	000112-37-8	60



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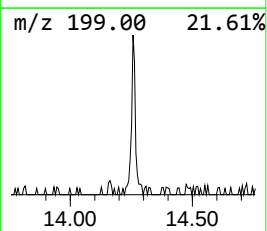
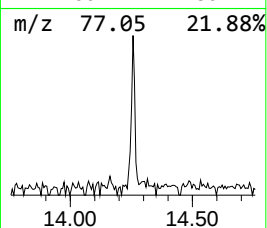
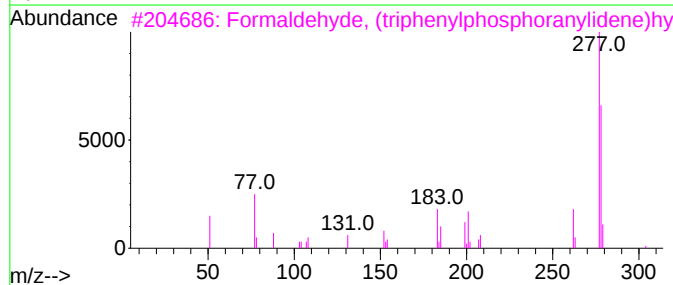
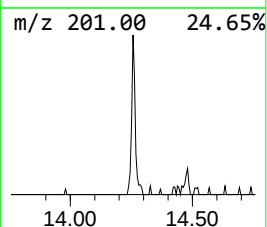
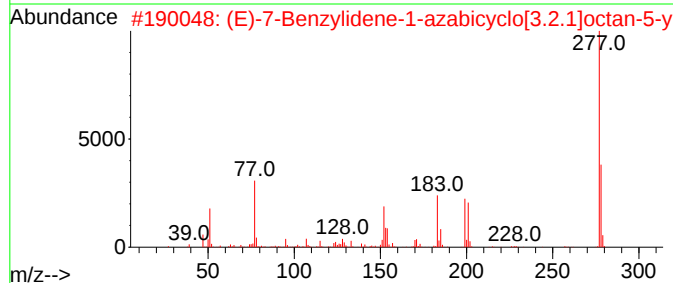
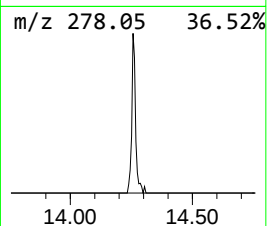
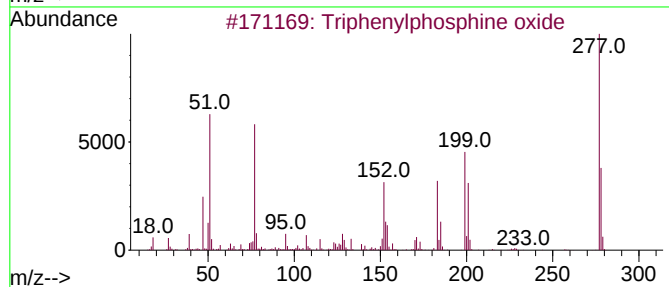
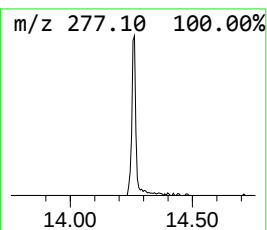
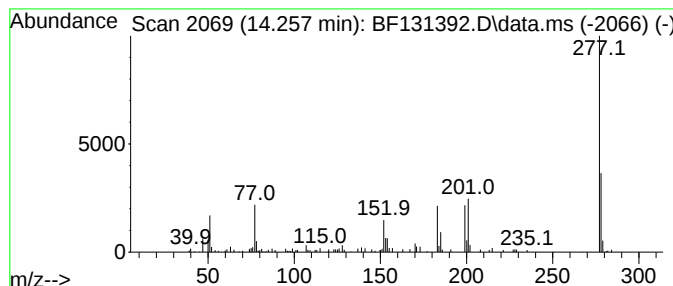
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Triphenylphosphine oxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.257	3.04 ng	79887	Chrysene-d12	14.163

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	96
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	91
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	45
4			Cobalt, (.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	38
5			Oxoprophines	277	C17H11N03	1000128-51-1	9



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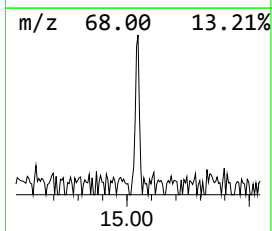
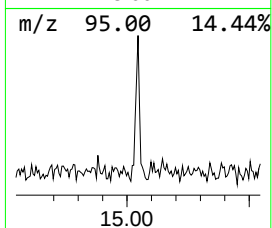
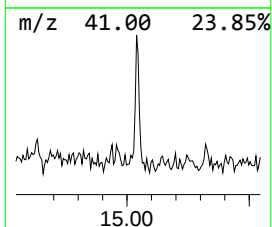
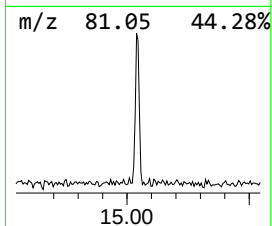
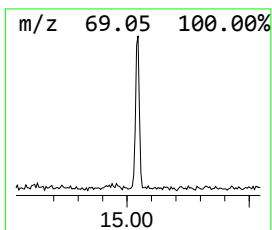
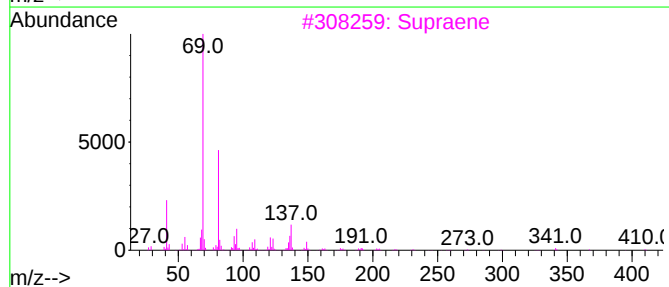
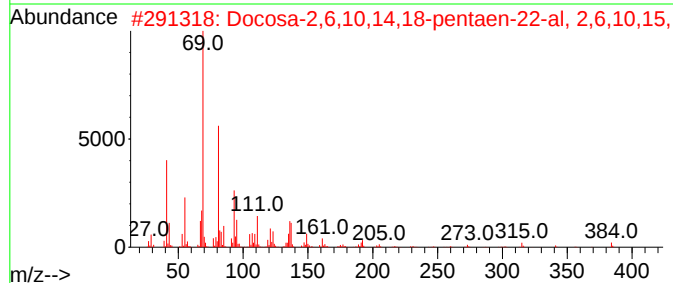
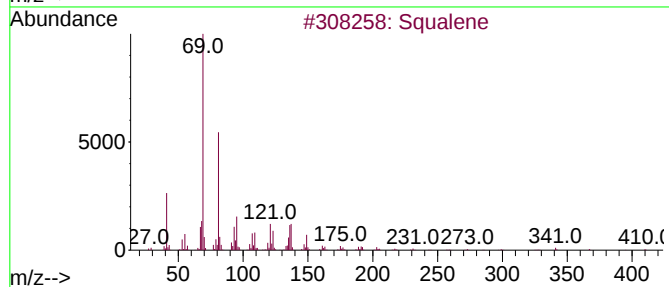
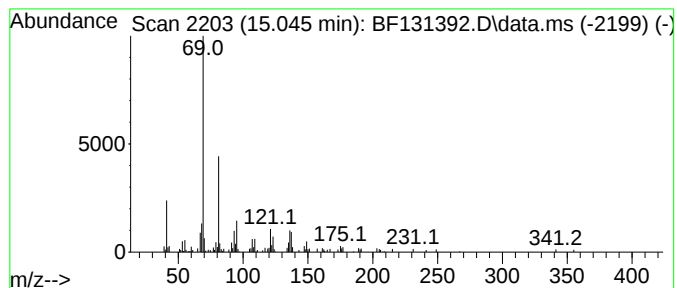
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.045	2.57 ng	69498	Perylene-d12	15.704

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	91
2			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	90
3			Supraene	410	C30H50	007683-64-9	86
4			.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	78
5			2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112522\
Data File : BF131392.D
Acq On : 25 Nov 2022 12:54
Operator : CG\JU
Sample : N5742-09
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-45

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.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
Butane, 2-metho...	2.299	80.4	ng	2403320	1	6.957	598028	20.0
2-Pentanone, 4-...	5.181	8.6	ng	256045	1	6.957	598028	20.0
n-Hexadecanoic ...	12.033	21.0	ng	901875	4	11.504	858379	20.0
Octadecanoic acid	12.827	38.5	ng	1650150	4	11.504	858379	20.0
Triphenylphosph...	14.257	3.0	ng	79887	5	14.163	526273	20.0
Squalene	15.045	2.6	ng	69498	6	15.704	539831	20.0