

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050823\
 Data File : BF133302.D
 Acq On : 08 May 2023 19:08
 Operator : CG\JU
 Sample : 02660-01
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WATER-SAMPLE-API-3-5

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-BF042123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133302.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.899	474	478	486	rVB	650282	725785	11.60%	2.005%
2	5.328	547	551	555	rBV	2882648	2646593	42.31%	7.312%
3	5.728	615	619	625	rBV	118259	116090	1.86%	0.321%
4	6.357	722	726	734	rBV	2028937	1611602	25.76%	4.453%
5	6.722	784	788	791	rBV	1393312	1204153	19.25%	3.327%
6	6.781	795	798	804	rVB2	76600	64084	1.02%	0.177%
7	7.287	878	884	887	rBV	3749884	3865653	61.80%	10.680%
8	7.404	898	904	908	rVB	198436	234074	3.74%	0.647%
9	8.004	1002	1006	1009	rBV	2130640	1588371	25.39%	4.388%
10	9.086	1185	1190	1192	rBV	6216328	6255150	100.00%	17.282%
11	9.610	1277	1279	1282	rBV2	92698	109478	1.75%	0.302%
12	9.657	1285	1287	1291	rVB	112501	88051	1.41%	0.243%
13	9.757	1300	1304	1307	rBV	2059229	1744756	27.89%	4.820%
14	9.816	1312	1314	1317	rBV3	70739	68390	1.09%	0.189%
15	9.981	1339	1342	1347	rBV6	64590	109317	1.75%	0.302%
16	10.022	1347	1349	1351	rBV2	104720	78265	1.25%	0.216%
17	10.257	1386	1389	1395	rVB4	207748	232270	3.71%	0.642%
18	10.310	1395	1398	1399	rBV2	109016	112364	1.80%	0.310%
19	10.381	1407	1410	1412	rBV4	118939	139741	2.23%	0.386%
20	10.469	1423	1425	1429	rBV	238575	239946	3.84%	0.663%
21	10.551	1434	1439	1441	rVV	3317386	3293999	52.66%	9.101%
22	11.080	1527	1529	1531	rBV2	123668	109859	1.76%	0.304%
23	11.239	1552	1556	1559	rVB	1852575	1503351	24.03%	4.153%
24	11.786	1645	1649	1655	rBV2	897555	938800	15.01%	2.594%
25	12.569	1778	1782	1793	rVB	1732703	1919887	30.69%	5.304%
26	12.827	1822	1826	1829	rBV	4740039	4550337	72.75%	12.572%
27	13.739	1978	1981	1990	rVB2	205901	298023	4.76%	0.823%
28	13.874	2000	2004	2007	rVB	1048130	954160	15.25%	2.636%
29	13.974	2019	2021	2028	rVB	293823	301947	4.83%	0.834%
30	15.292	2240	2245	2250	rVB	965995	1090367	17.43%	3.012%

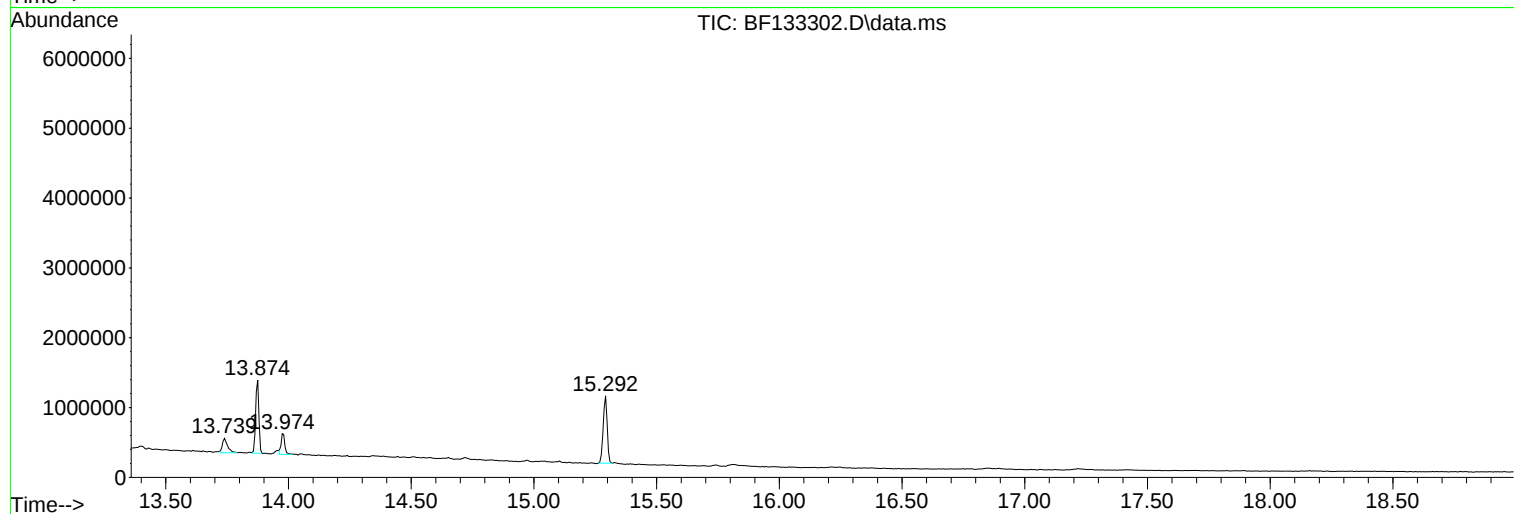
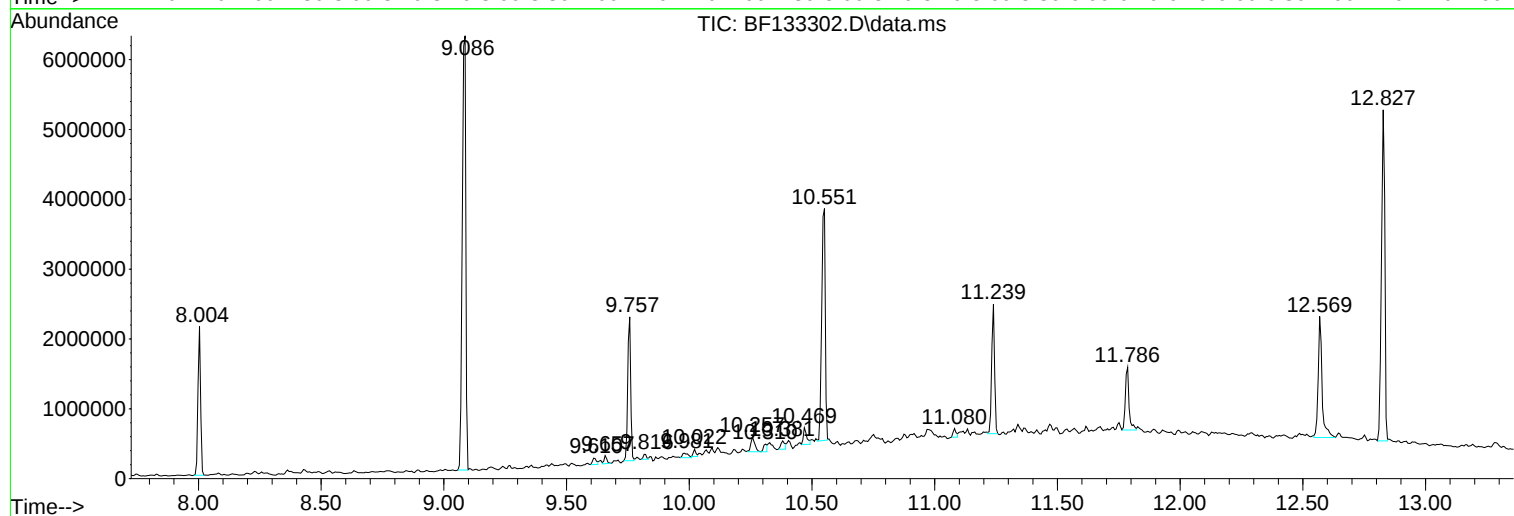
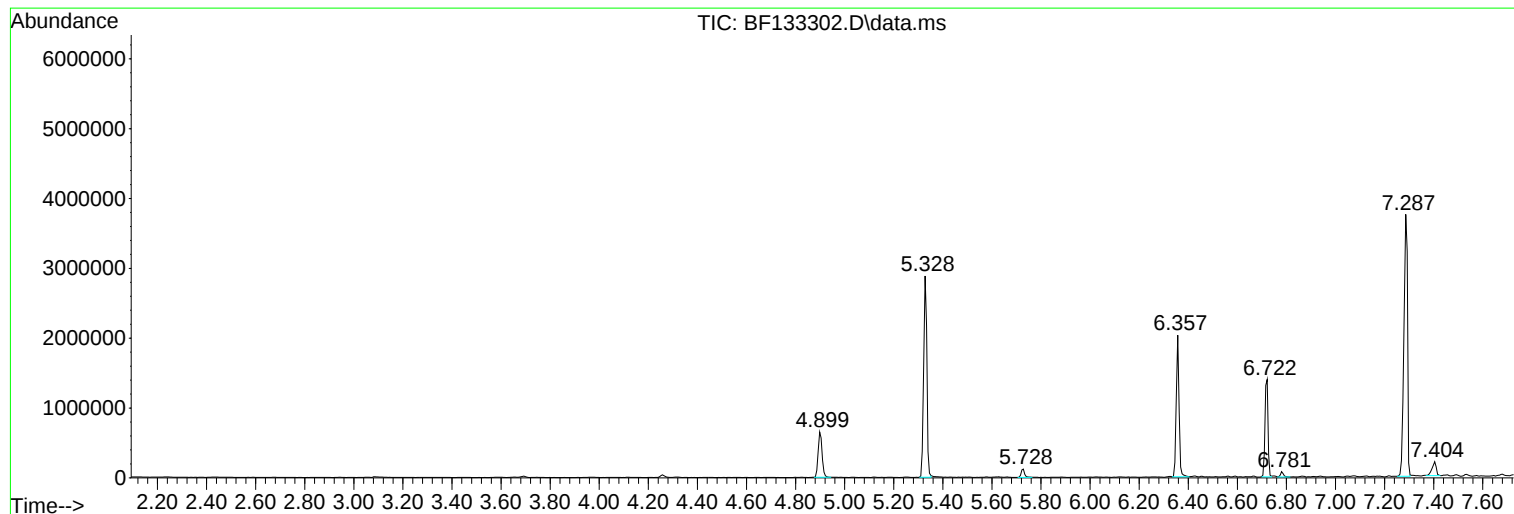
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WATER-SAMPLE-API-3-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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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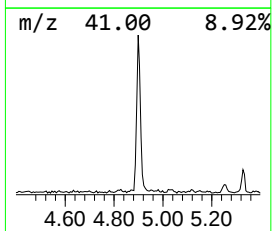
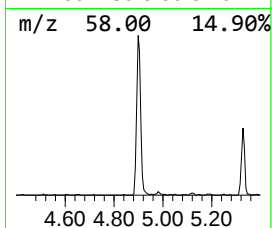
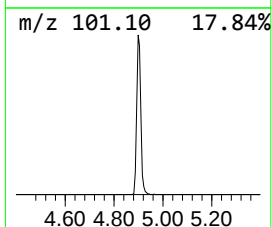
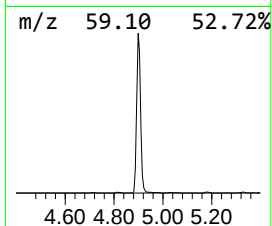
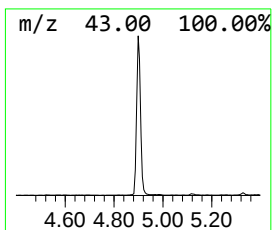
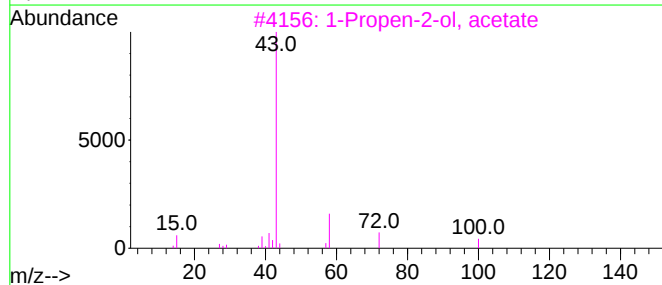
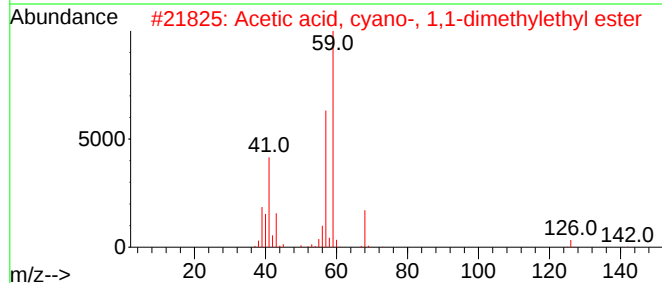
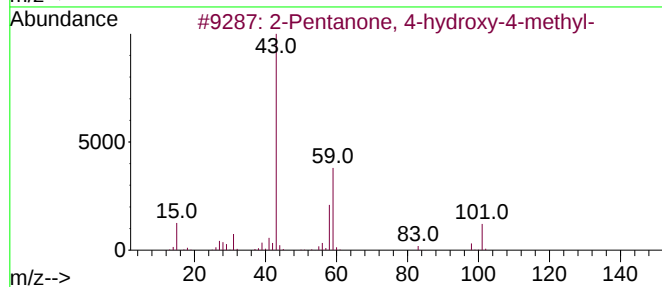
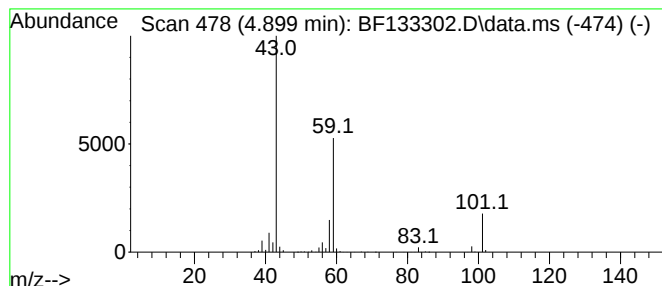
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.899	12.05 ng	725785	1,4-Dichlorobenzene-d4	6.722

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		
5	Allyl acetate	100	C5H8O2	000591-87-7	9		



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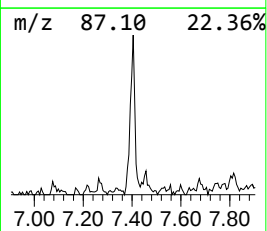
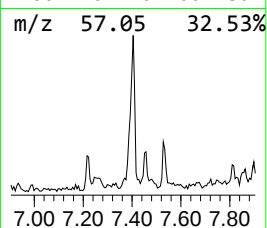
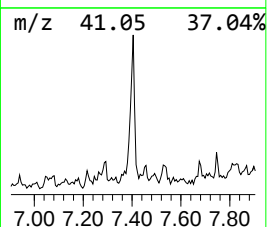
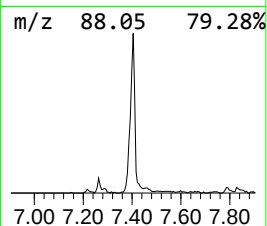
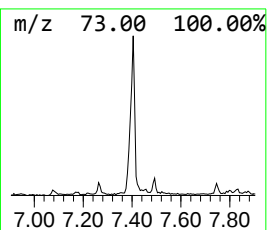
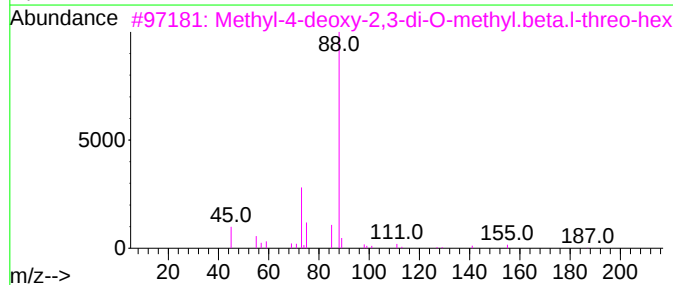
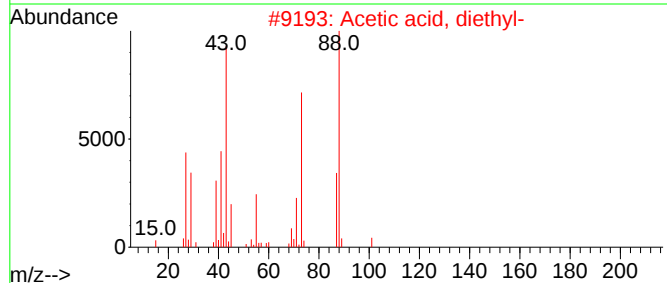
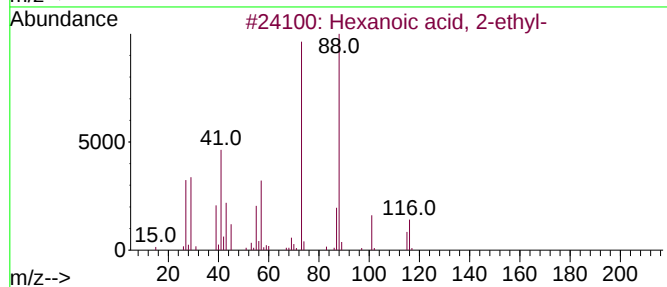
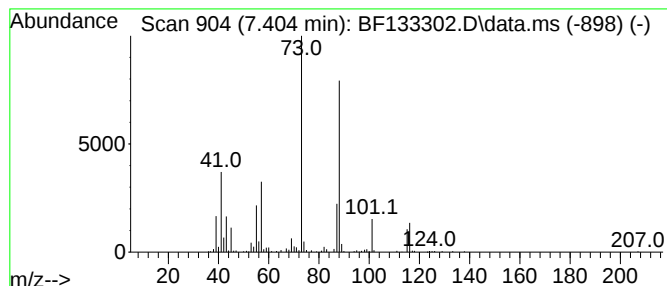
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 2 Hexanoic acid, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.404	2.95 ng	234074	Naphthalene-d8	8.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2			Acetic acid, diethyl-	116	C6H12O2	000088-09-5	59
3			Methyl-4-deoxy-2,3-di-O-methyl.b...	218	C9H14O6	1000312-09-9	50
4			Heptanoic acid, 2-methyl-, methy...	158	C9H18O2	051209-78-0	38
5			Heptanoic acid, 2,6-dimethyl-, m...	172	C10H20O2	033315-72-9	38



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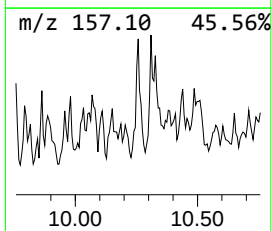
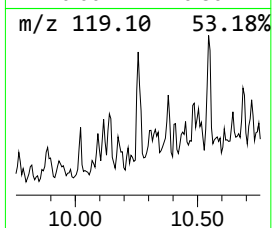
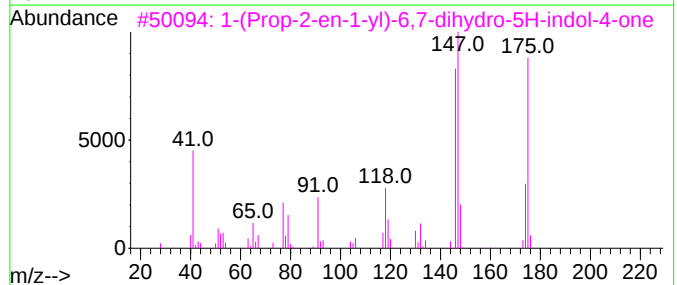
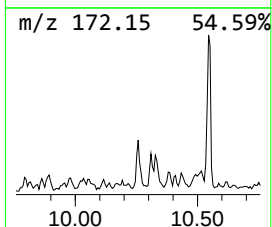
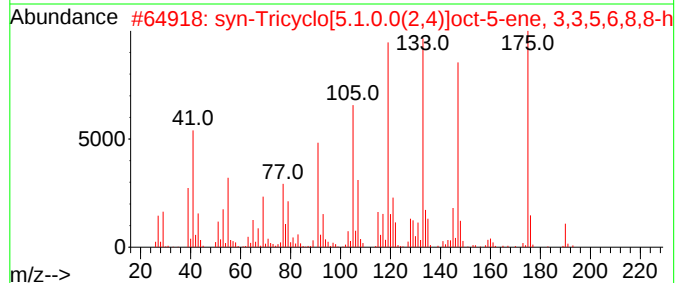
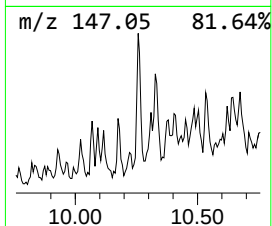
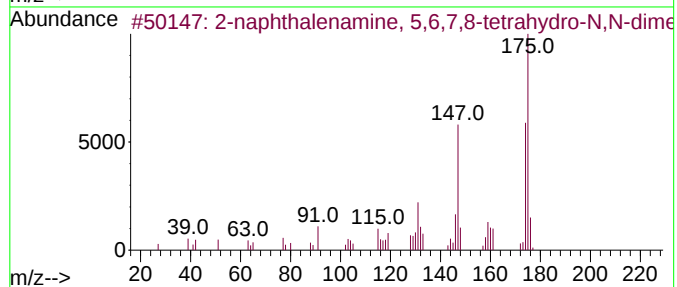
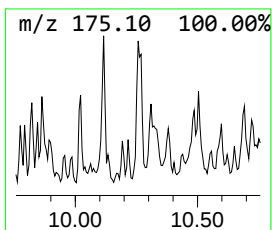
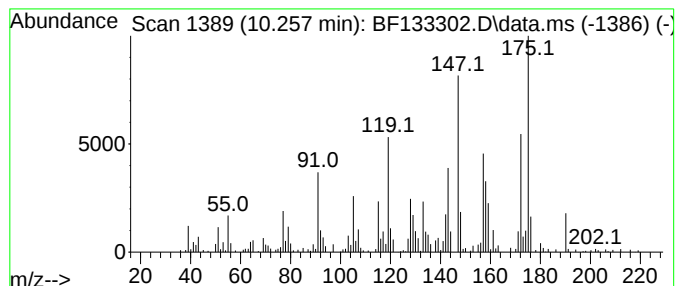
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Peak Number 3 unknown10.257 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.257	2.66 ng	232270	Acenaphthene-d10	9.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-naphthalenamine, 5,6,7,8-tetra...	175	C12H17N	1010404-71-6	45		
2	syn-Tricyclo[5.1.0.0(2,4)]oct-5-...	190	C14H22	1000161-99-5	38		
3	1-(Prop-2-en-1-yl)-6,7-dihydro-5...	175	C11H13NO	081565-17-5	30		
4	1,3,5-Cycloheptatriene, 2,4-diet...	176	C13H20	1000156-99-6	20		
5	1-Naphthalenamine, 5,6,7,8-tetra...	147	C10H13N	002217-41-6	18		



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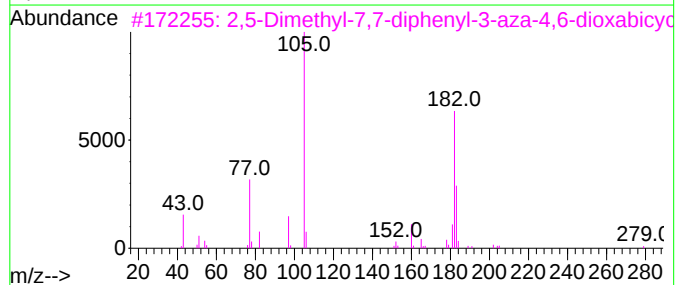
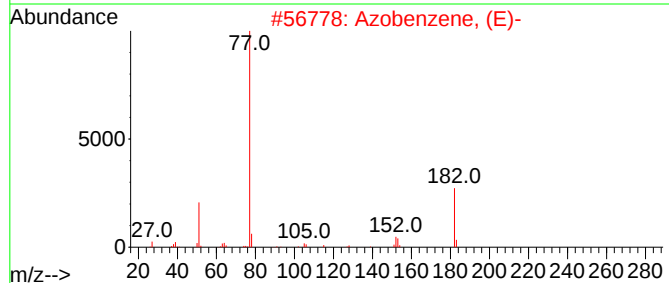
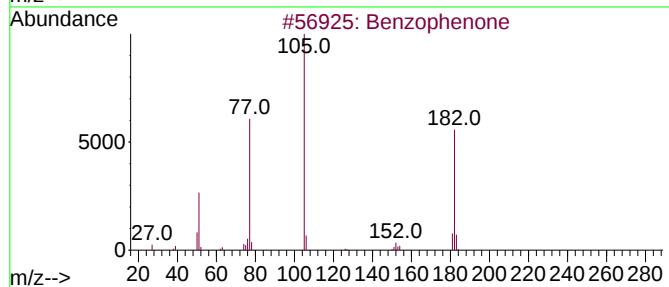
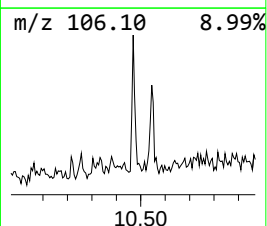
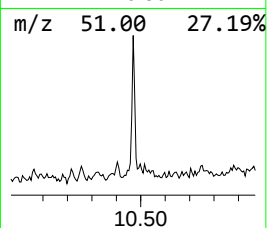
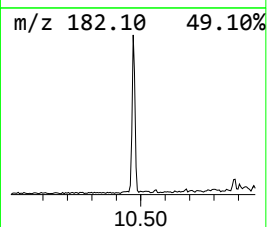
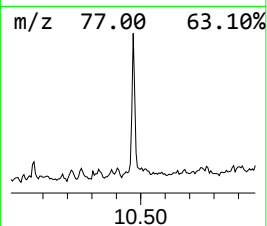
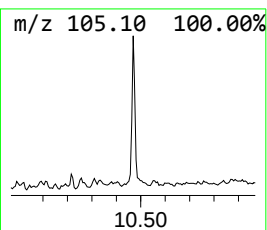
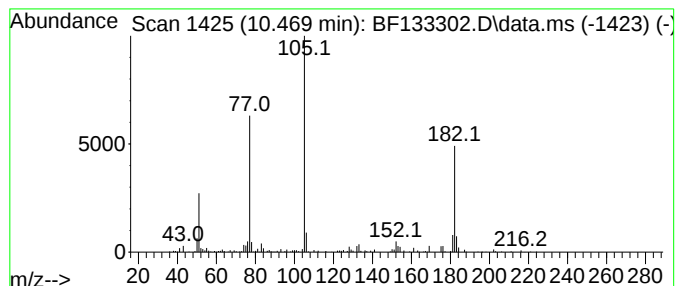
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Peak Number 4 Benzophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.469	2.75 ng	239946	Acenaphthene-d10	9.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Azobenzene, (E)-	182	C12H10N2	017082-12-1	59
3			2,5-Dimethyl-7,7-diphenyl-3-aza-...	279	C18H17NO2	078950-91-1	59
4			Benzoic acid, pentafluorophenyl ...	288	C13H5F5O2	1000360-67-9	47
5			Benzoylformic acid	150	C8H6O3	000611-73-4	46



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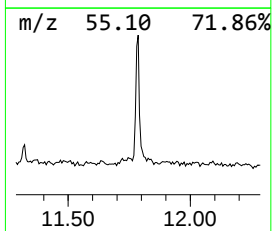
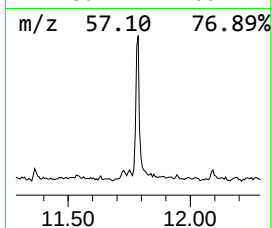
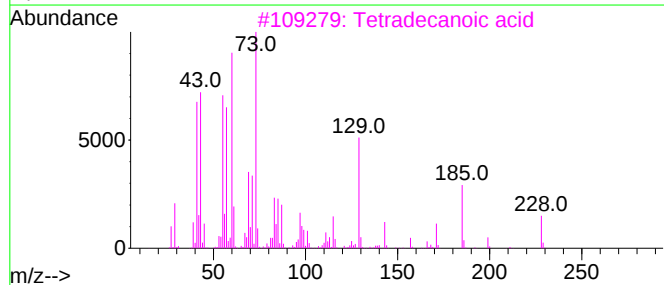
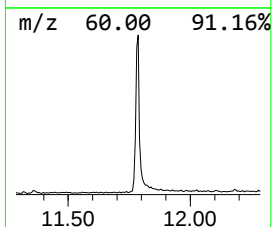
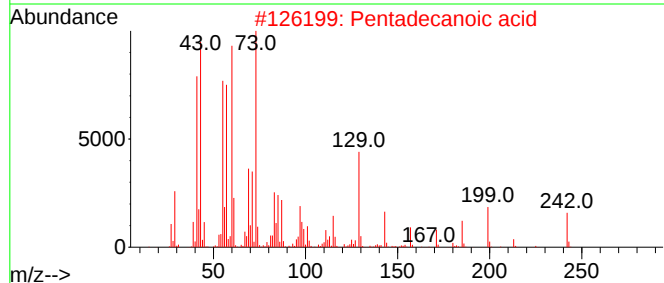
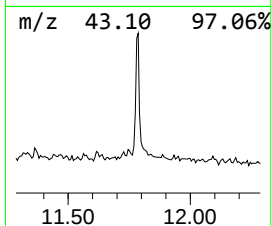
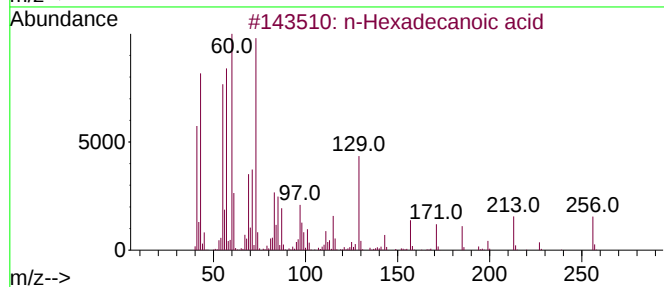
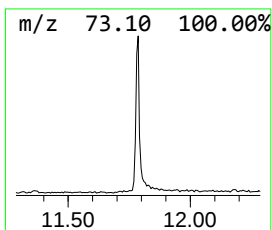
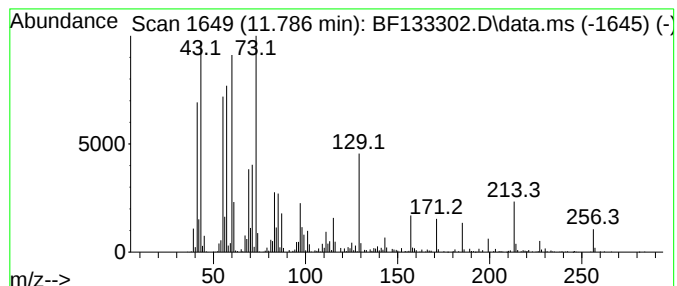
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.786	12.49 ng	938800	Phenanthrene-d10	11.239

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			n-Decanoic acid	172	C10H20O2	000334-48-5	70
5			Tridecanoic acid	214	C13H26O2	000638-53-9	64



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ClientSampleId :
WATER-SAMPLE-API-3-5

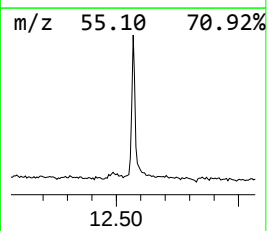
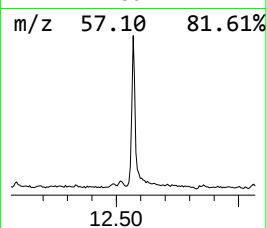
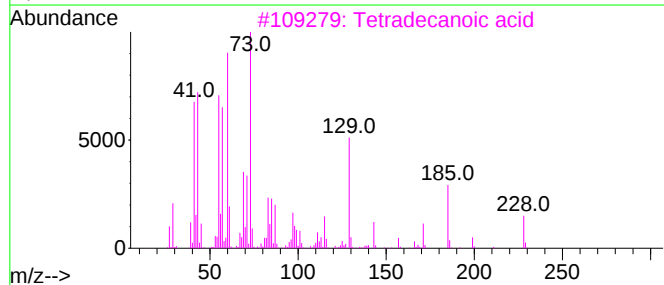
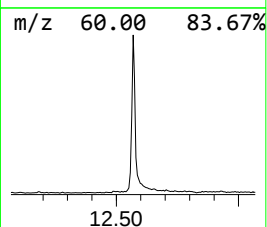
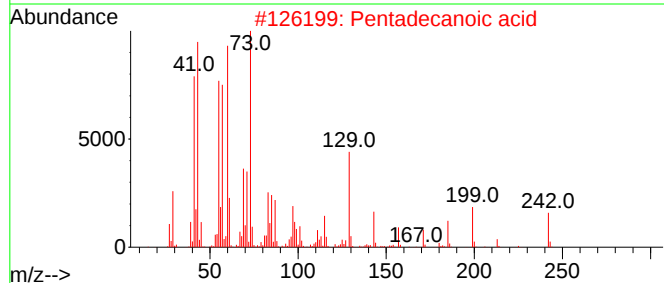
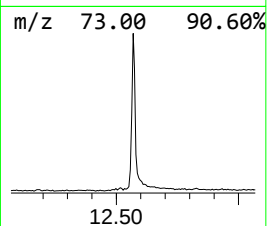
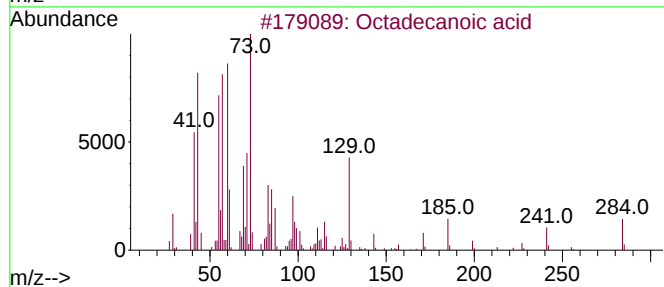
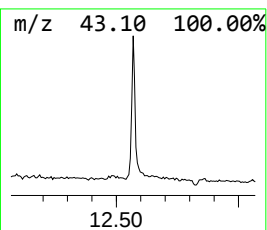
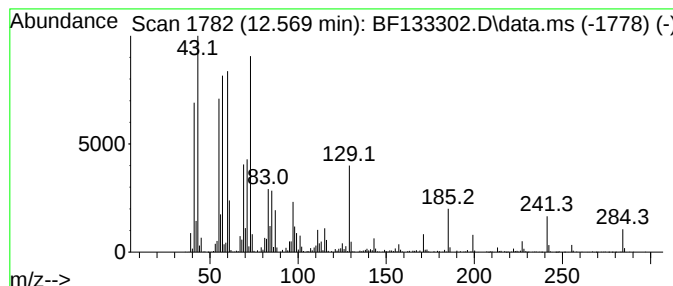
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.569	40.24 ng	1919890	Chrysene-d12	13.874

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72
5			n-Decanoic acid	172	C10H20O2	000334-48-5	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050823\
Data File : BF133302.D
Acq On : 08 May 2023 19:08
Operator : CG\JU
Sample : 02660-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WATER-SAMPLE-API-3-5

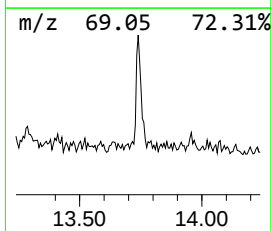
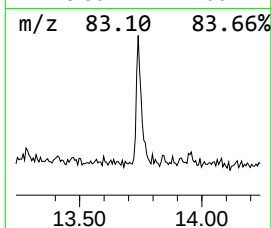
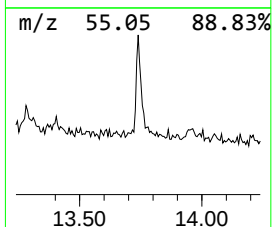
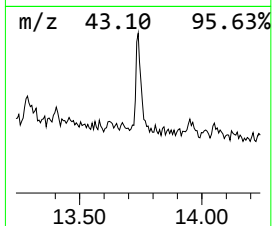
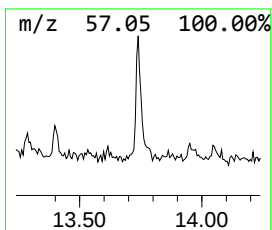
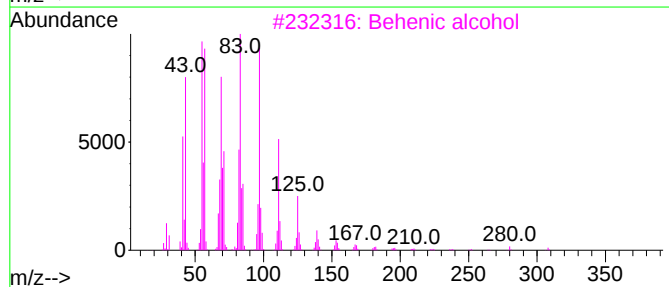
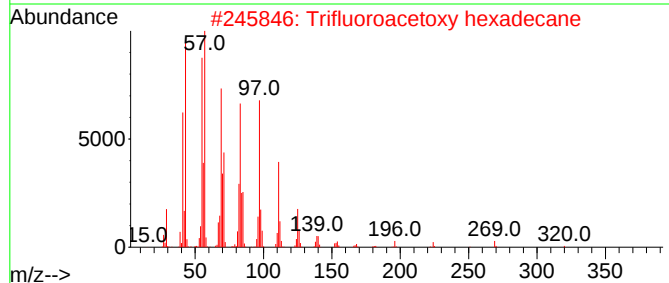
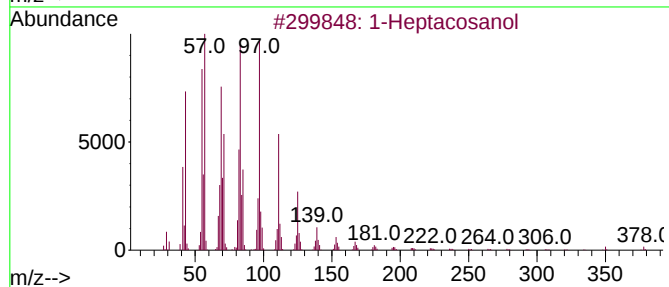
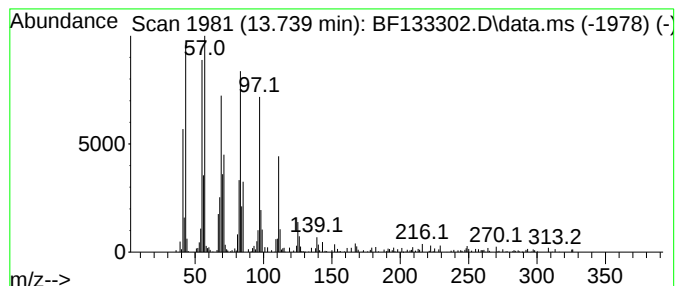
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Heptacosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.739	6.25 ng	298023	Chrysene-d12	13.874

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heptacosanol	396	C27H56O	002004-39-9	91
2			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
3			Behenic alcohol	326	C22H46O	000661-19-8	91
4			2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91
5			1-Tetracosene	336	C24H48	010192-32-2	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050823\
Data File : BF133302.D
Acq On : 08 May 2023 19:08
Operator : CG\JU
Sample : 02660-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WATER-SAMPLE-API-3-5

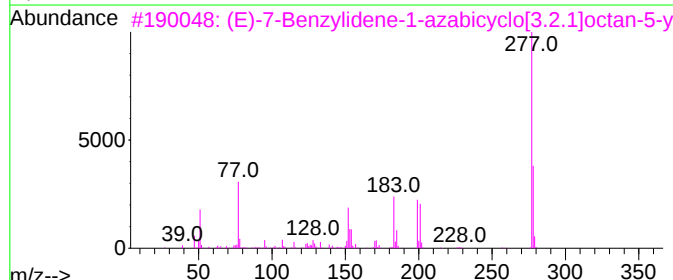
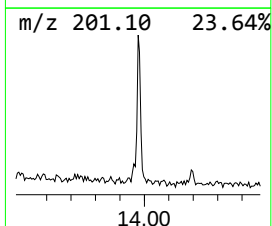
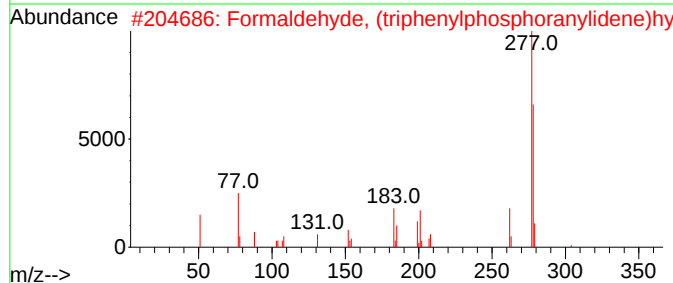
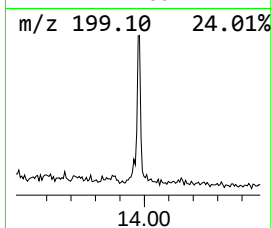
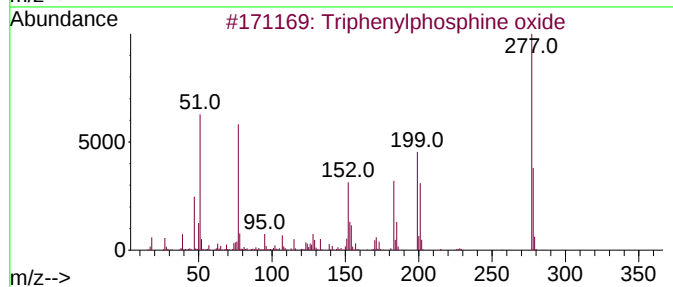
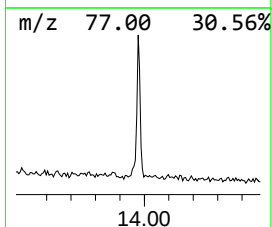
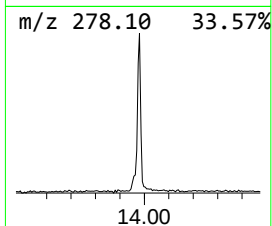
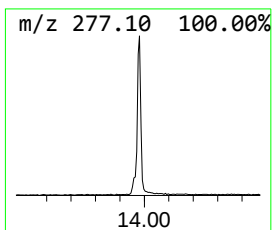
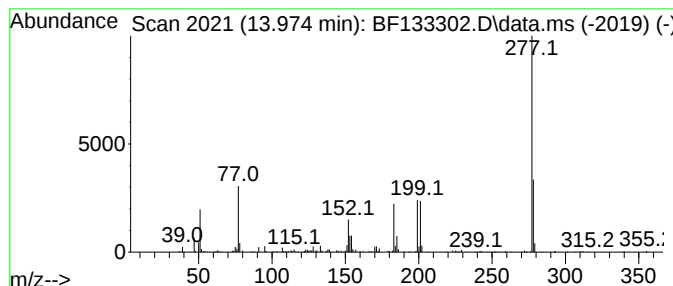
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Triphenylphosphine oxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.974	6.33 ng	301947	Chrysene-d12	13.874

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	64
2			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50
3			(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19N03S	1000483-83-4	46
4			4-Nitro-4'-methyldiphenylsulfone	277	C13H11N04S	004094-37-5	43
5			(Carbethoxymethyl)-triphenylphos...	428	C22H22Br02P	001530-45-6	40



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050823\
Data File : BF133302.D
Acq On : 08 May 2023 19:08
Operator : CG\JU
Sample : 02660-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WATER-SAMPLE-API-3-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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-...	4.899	12.1	ng	725785	1	6.722	1204150	20.0
Hexanoic acid, ...	7.404	3.0	ng	234074	2	8.004	1588370	20.0
unknown10.257	10.257	2.7	ng	232270	3	9.757	1744760	20.0
Benzophenone	10.469	2.8	ng	239946	3	9.757	1744760	20.0
n-Hexadecanoic ...	11.786	12.5	ng	938800	4	11.239	1503350	20.0
Octadecanoic acid	12.569	40.2	ng	1919890	5	13.874	954160	20.0
1-Heptacosanol	13.739	6.3	ng	298023	5	13.874	954160	20.0
Triphenylphosph...	13.974	6.3	ng	301947	5	13.874	954160	20.0