

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021723\
 Data File : BF132463.D
 Acq On : 17 Feb 2023 22:16
 Operator : CG\JU
 Sample : 01595-04
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S-655-1

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-BF021623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132463.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.266	408	413	421	rVB	1986955	2505157	41.96%	4.935%
2	5.648	473	478	482	rBV	4762130	5070015	84.92%	9.987%
3	6.642	641	647	650	rBV	4649897	5071126	84.94%	9.989%
4	7.019	708	711	715	rVB	1843431	1509639	25.29%	2.974%
5	7.583	802	807	810	rBV	3496552	3347081	56.06%	6.593%
6	8.307	926	930	933	rBV	2386039	1942886	32.54%	3.827%
7	9.383	1107	1113	1116	rBV	6269159	5692353	95.35%	11.213%
8	10.072	1226	1230	1233	rBV	2624912	2246805	37.63%	4.426%
9	10.783	1347	1351	1355	rBV	3042016	2745774	45.99%	5.409%
10	10.866	1360	1365	1368	rBV	3984151	3803871	63.72%	7.493%
11	11.095	1400	1404	1409	rBV	469064	412058	6.90%	0.812%
12	11.160	1411	1415	1418	rVV	170076	159656	2.67%	0.314%
13	11.460	1463	1466	1469	rVB	103214	74483	1.25%	0.147%
14	11.566	1480	1484	1487	rBV	2763505	2366936	39.65%	4.662%
15	12.077	1567	1571	1588	rBV2	1073588	1259356	21.09%	2.481%
16	12.330	1611	1614	1621	rVB	100611	100007	1.68%	0.197%
17	12.636	1659	1666	1671	rBV4	37121	84475	1.41%	0.166%
18	12.789	1686	1692	1700	rBV7	32412	74525	1.25%	0.147%
19	12.866	1701	1705	1718	rBV	301693	407931	6.83%	0.804%
20	13.160	1750	1755	1758	rBV	6075911	5970002	100.00%	11.760%
21	14.048	1901	1906	1908	rBV2	153944	198020	3.32%	0.390%
22	14.077	1908	1911	1918	rVB	203714	256480	4.30%	0.505%
23	14.218	1931	1935	1939	rBV	2090628	1972565	33.04%	3.886%
24	14.312	1944	1951	1957	rBV	985813	1125429	18.85%	2.217%
25	14.360	1957	1959	1963	rVB	71608	64447	1.08%	0.127%
26	14.671	2009	2012	2019	rBV	77565	83356	1.40%	0.164%
27	15.001	2062	2068	2075	rVB2	66258	94956	1.59%	0.187%
28	15.089	2079	2083	2089	rVB	157734	174605	2.92%	0.344%
29	15.365	2127	2130	2136	rVB	57454	70811	1.19%	0.139%
30	15.777	2194	2200	2212	rBV	1298646	1815517	30.41%	3.576%
31	16.259	2278	2282	2290	rVB2	37741	65843	1.10%	0.130%

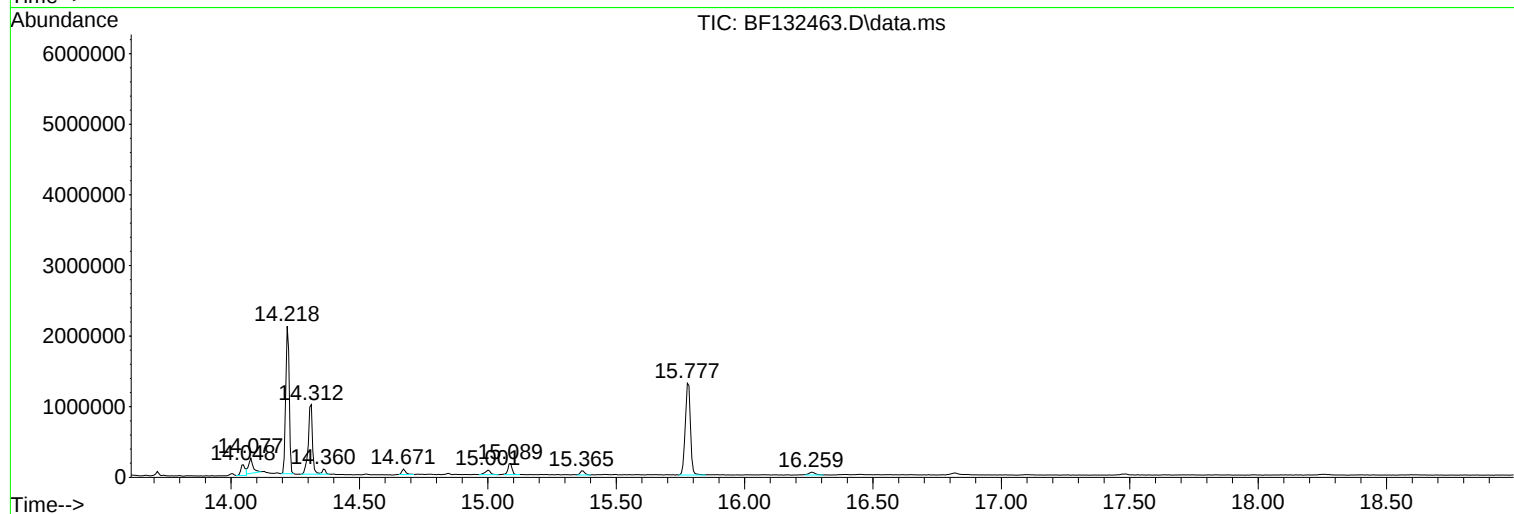
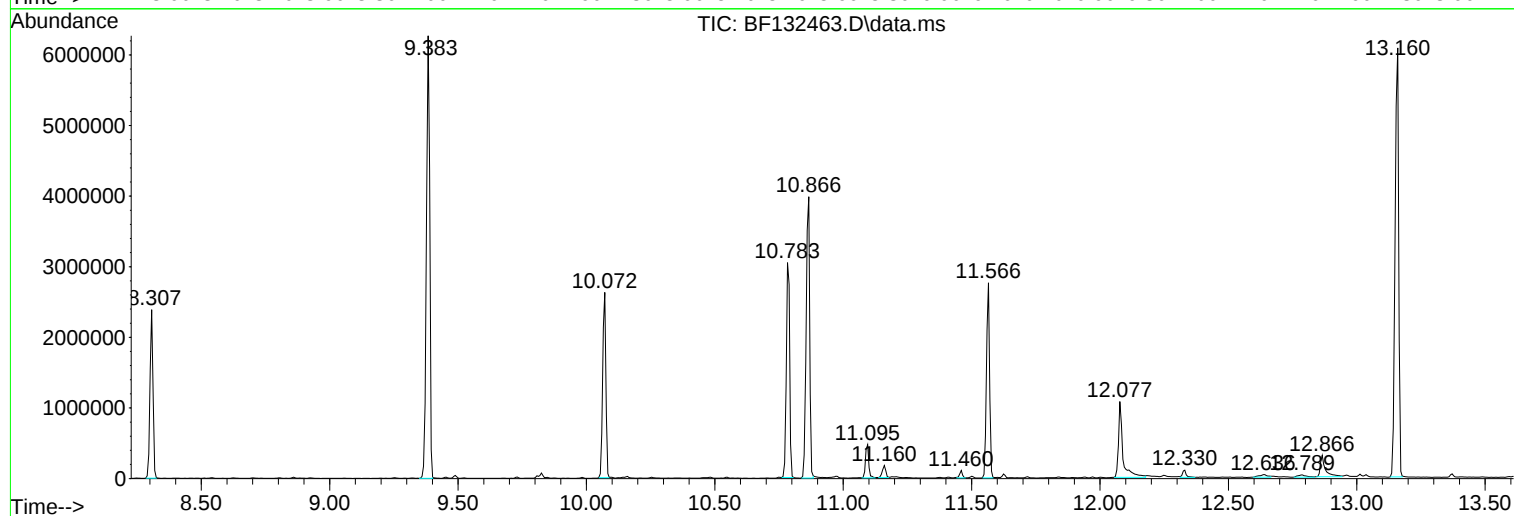
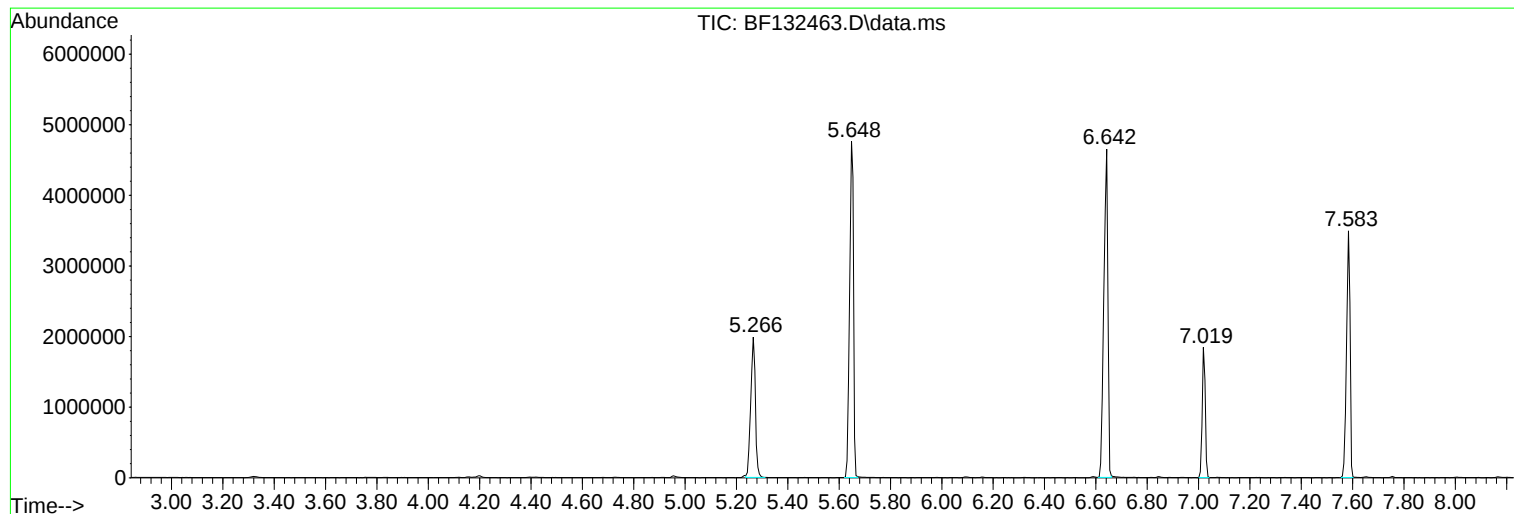
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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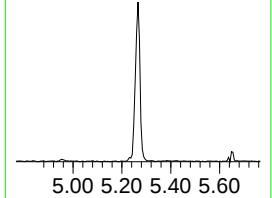
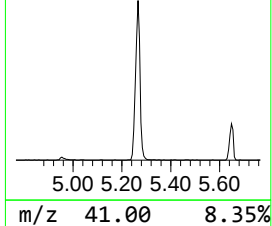
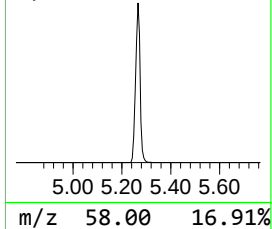
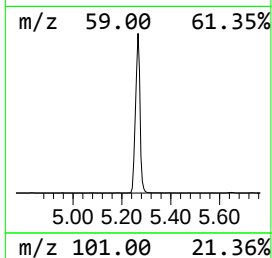
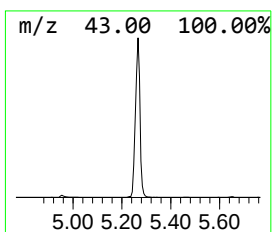
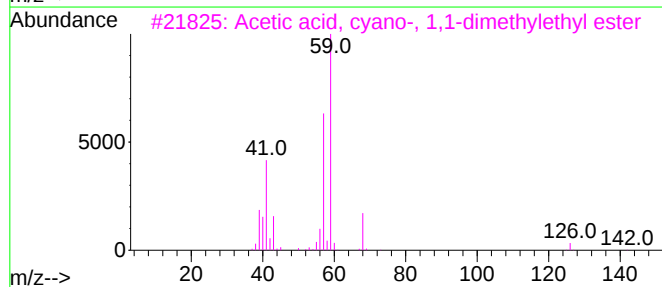
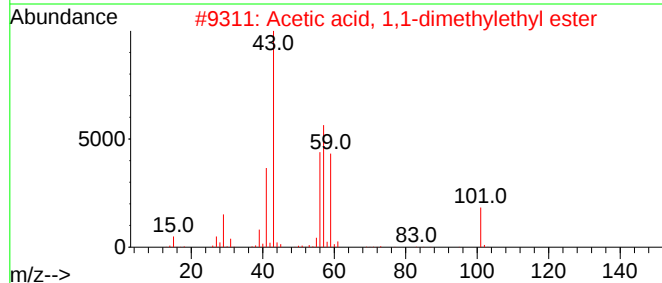
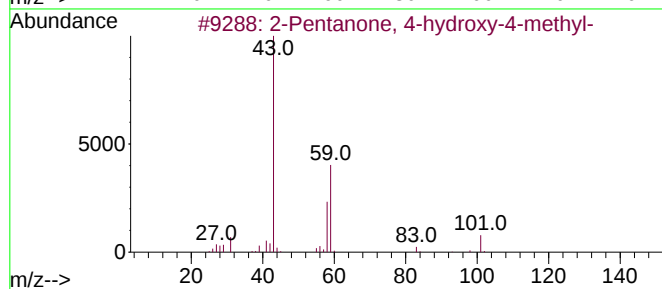
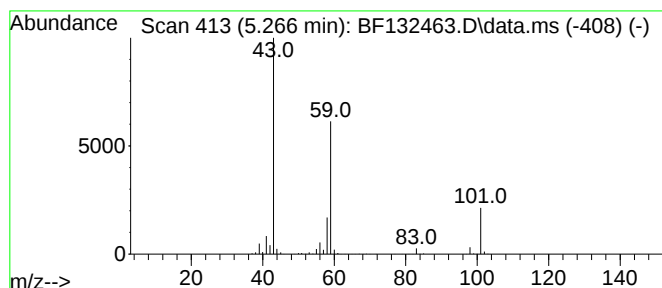
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021623.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.266	33.19 ng	2505160	1,4-Dichlorobenzene-d4	7.019

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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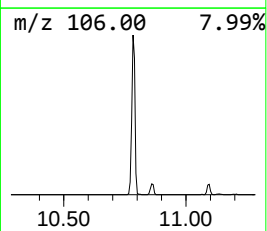
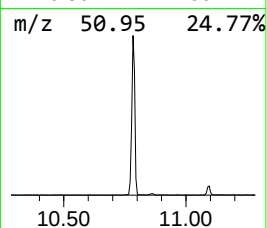
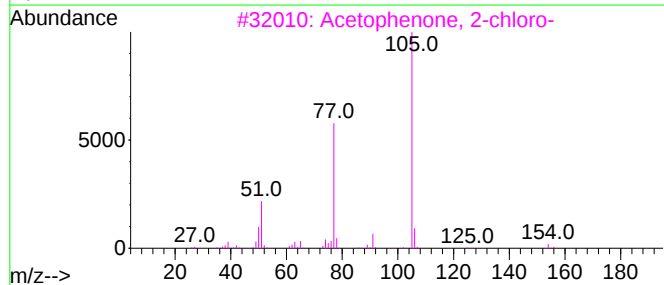
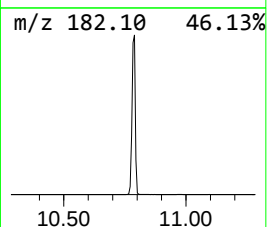
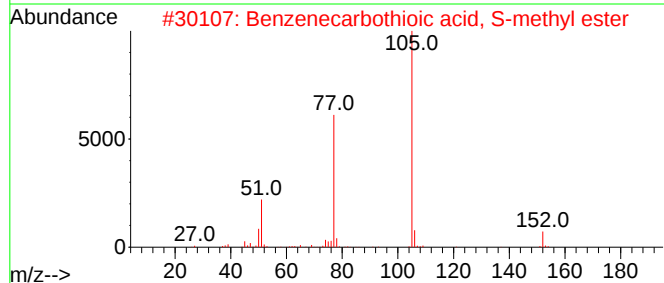
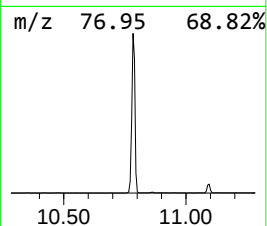
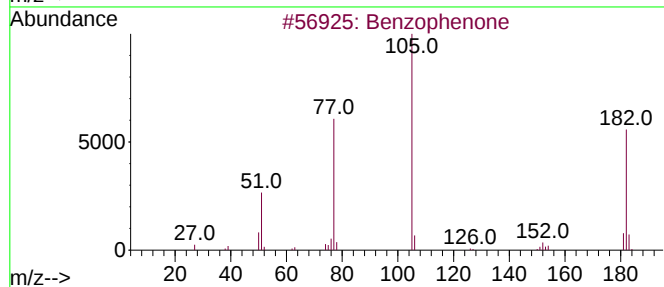
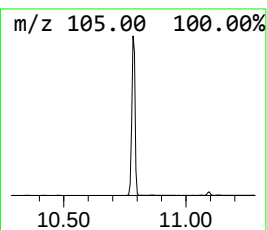
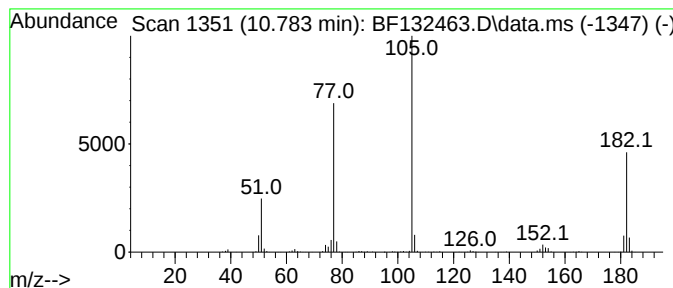
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Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.783	24.44 ng	2745770	Acenaphthene-d10	10.072

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	50
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
4			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	49
5			Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	47



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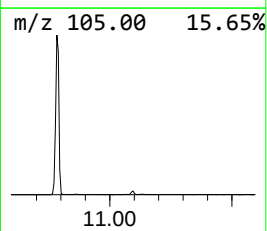
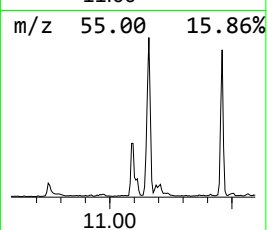
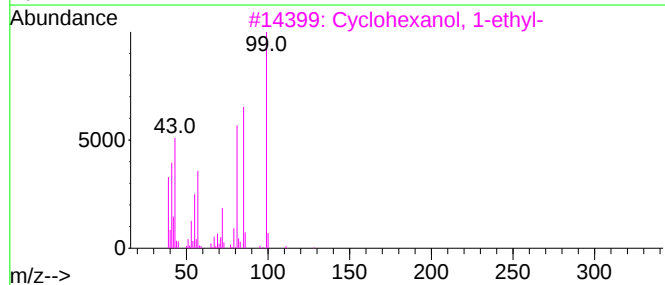
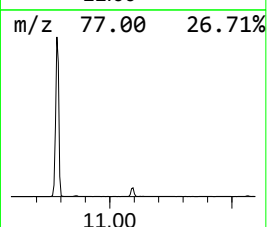
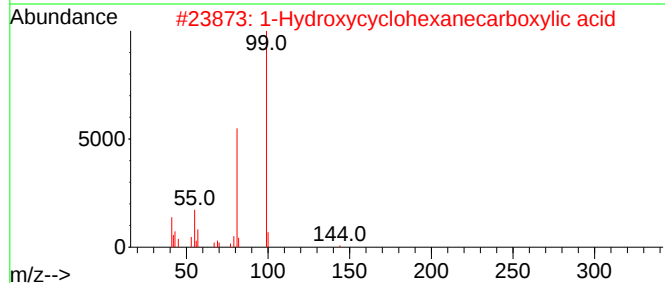
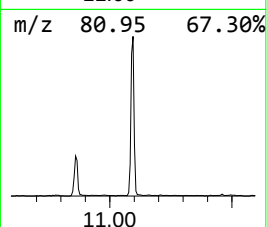
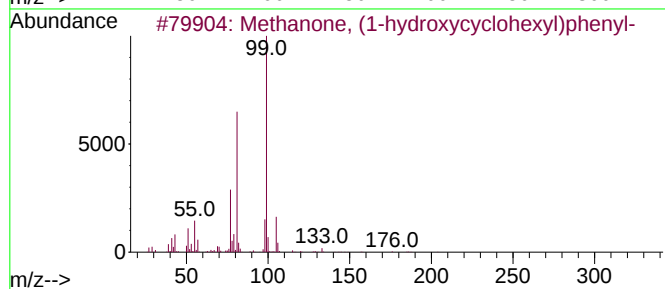
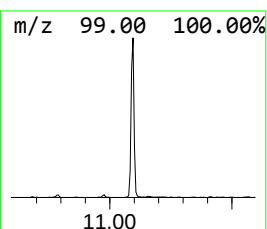
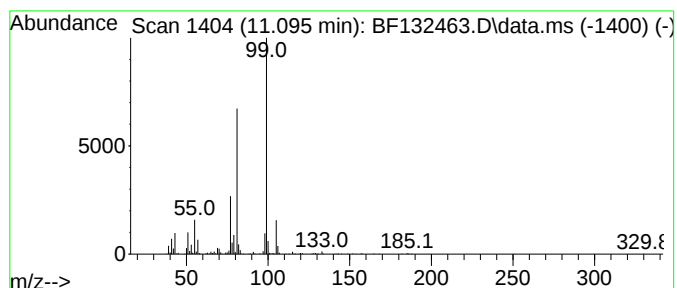
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Peak Number 3 Methanone, (1-hydroxycyclohexyl) Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.095	3.48 ng	412058	Phenanthrene-d10	11.566	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methanone, (1-hydroxycyclohexyl)...	204	C13H16O2	000947-19-3	53
2	1-Hydroxycyclohexanecarboxylic acid	144	C7H12O3	001123-28-0	47
3	Cyclohexanol, 1-ethyl-	128	C8H16O	001940-18-7	38
4	3,5-Diamino-1,2,4-triazole	99	C2H5N5	001455-77-2	37
5	Cholestan-22(26)-isoeopoxv-3.beta...	402	C27H46O2	103099-02-1	28



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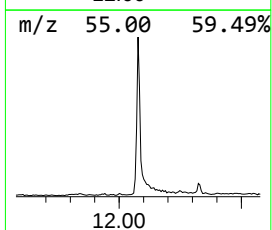
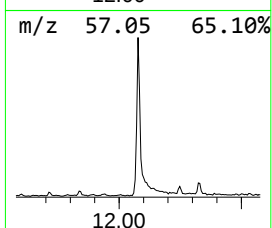
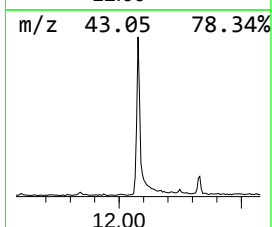
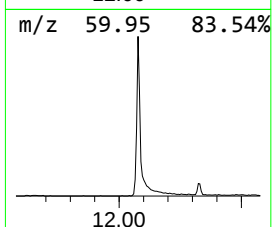
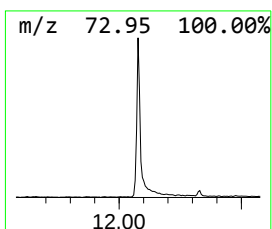
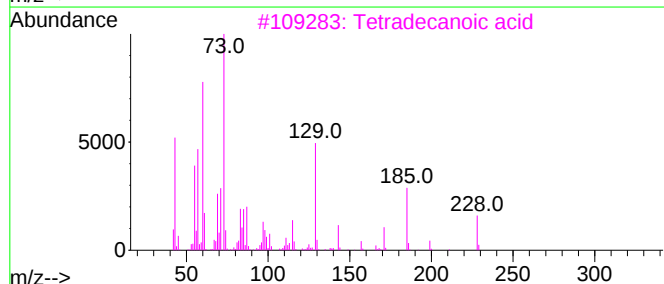
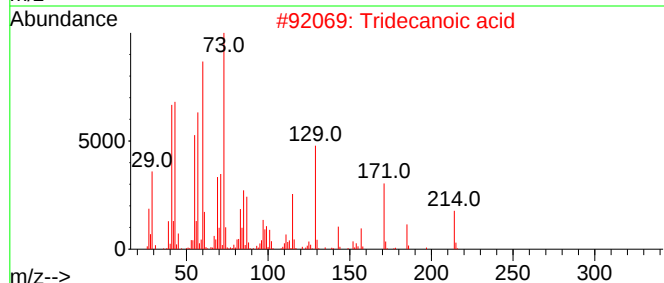
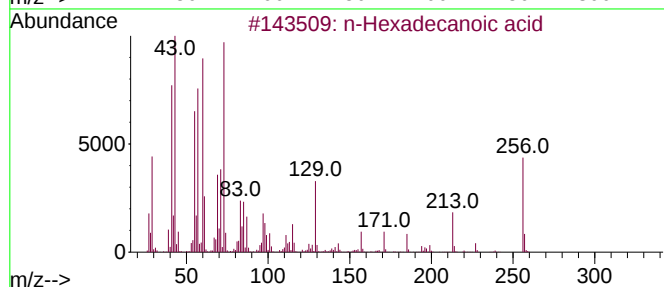
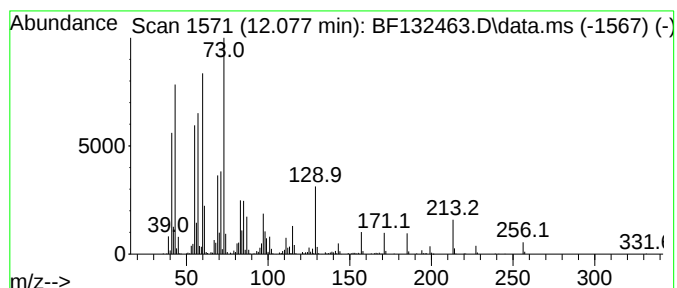
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.077	10.64 ng	1259360	Phenanthrene-d10	11.566

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	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5			Estra-1,3,5(10)-trien-17.β.-ol	256	C18H24O	002529-64-8	18



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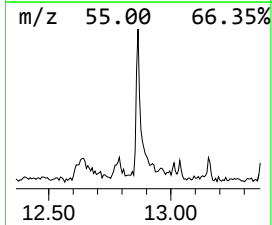
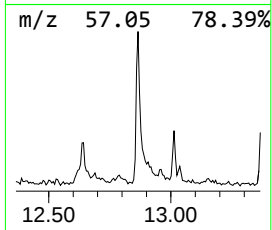
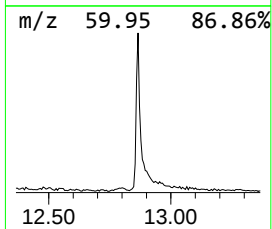
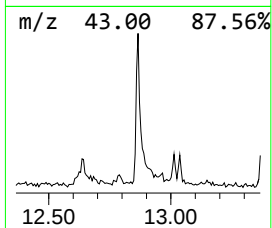
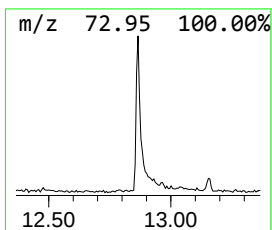
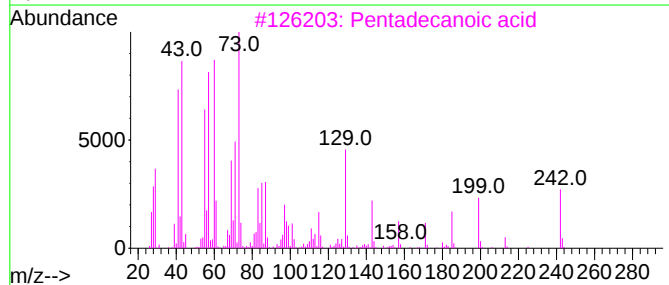
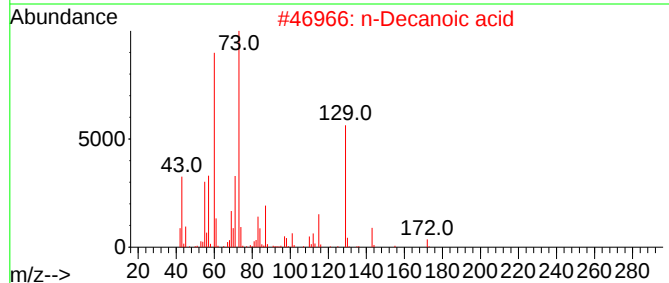
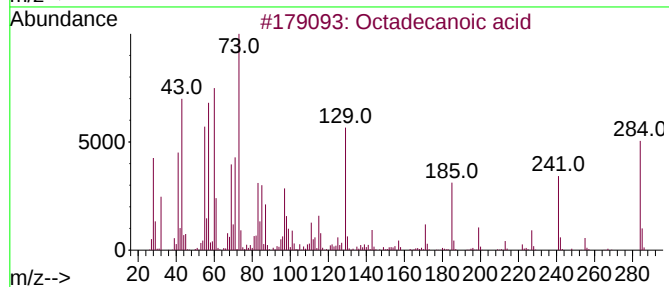
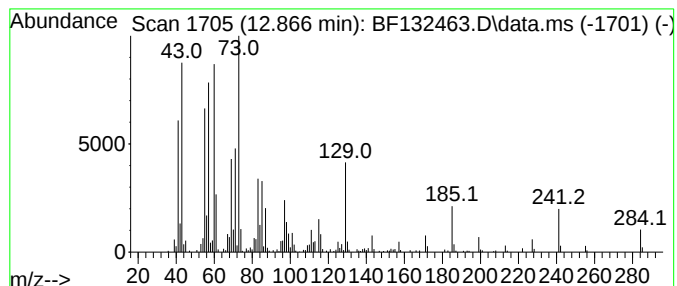
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Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.866	3.45 ng	407931	Phenanthrene-d10	11.566

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Decanoic acid	172	C10H20O2	000334-48-5	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			Tridecanoic acid	214	C13H26O2	000638-53-9	70



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ClientSampleId :
S-655-1

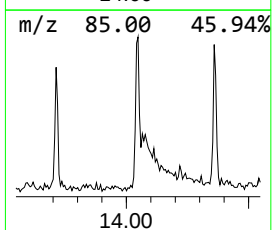
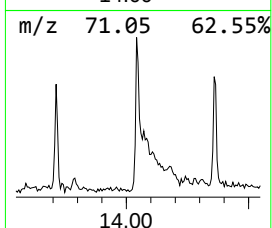
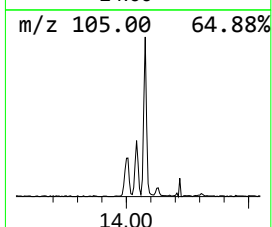
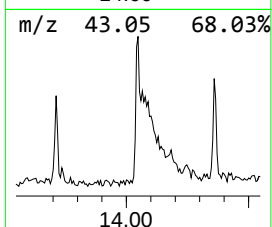
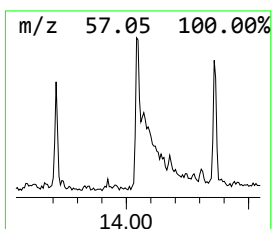
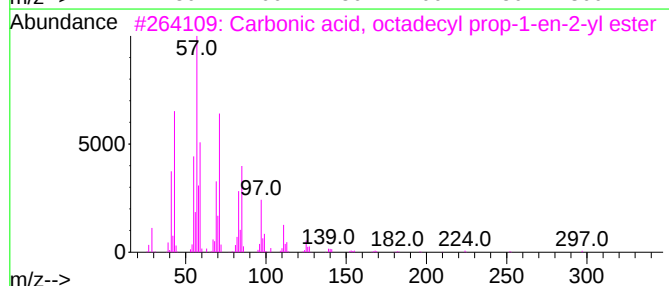
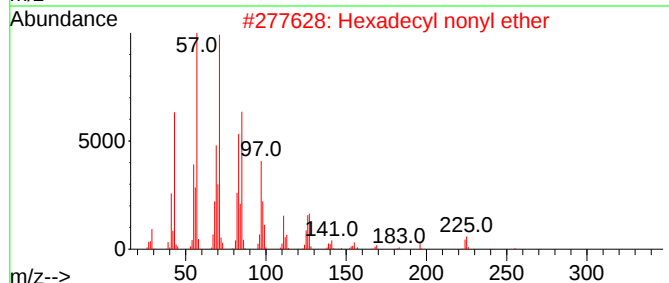
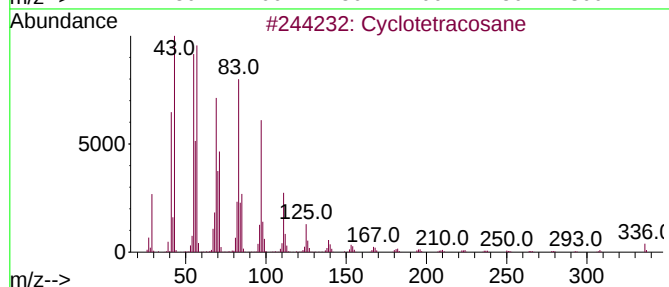
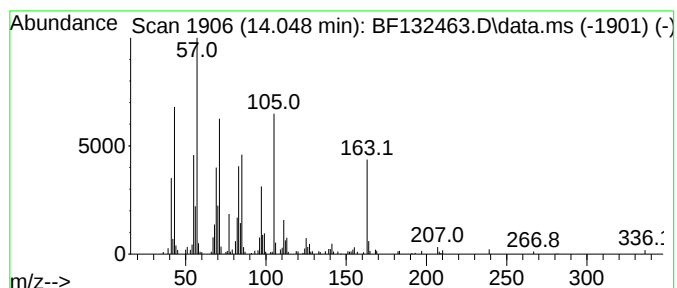
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cyclotetracosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.048	2.01 ng	198020	Chrysene-d12	14.218

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotetracosane	336	C24H48	000297-03-0	95
2			Hexadecyl nonyl ether	368	C25H52O	1000406-37-7	81
3			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	81
4			Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	76
5			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021723\
Data File : BF132463.D
Acq On : 17 Feb 2023 22:16
Operator : CG\JU
Sample : 01595-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

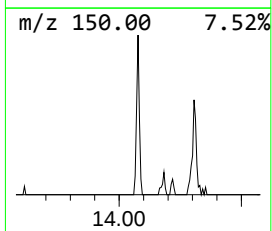
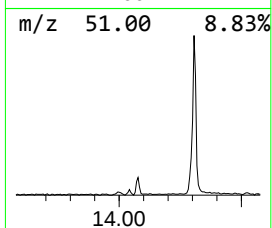
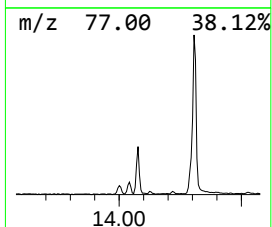
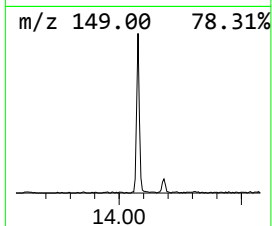
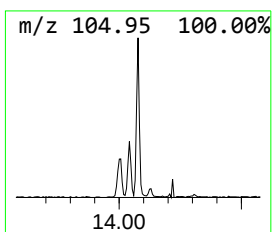
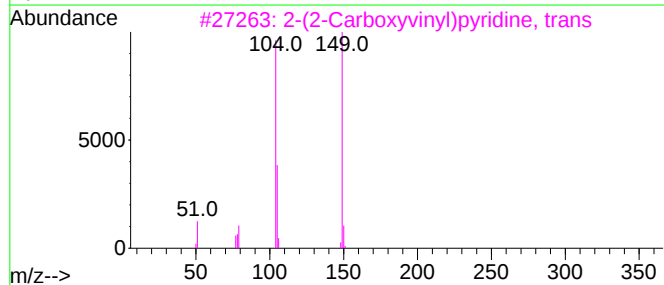
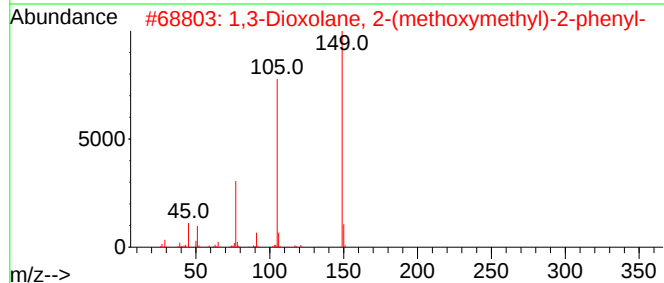
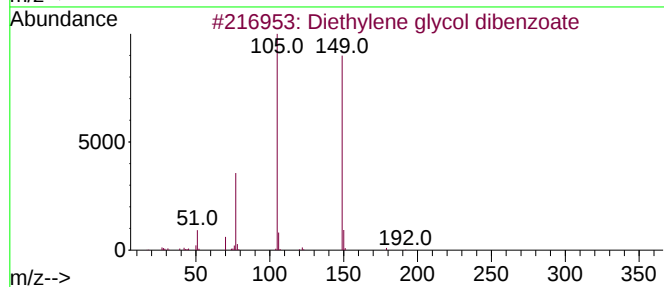
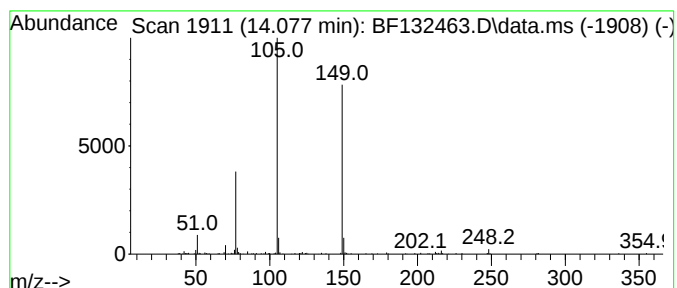
Instrument :
BNA_F
ClientSampleId :
S-655-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Diethylene glycol dibenzoate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.077	2.60 ng	256480	Chrysene-d12	14.218	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	86
2	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	50
3	2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	49
4	2,3-Dimethyl-4a,8a-diphenyl-hexa...	326	C20H22O4	1000297-07-0	38
5	Benzoic acid, 3-methylphenyl ester	212	C14H12O2	1000357-80-0	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021723\
Data File : BF132463.D
Acq On : 17 Feb 2023 22:16
Operator : CG\JU
Sample : 01595-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-655-1

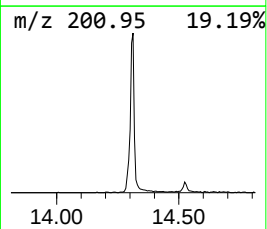
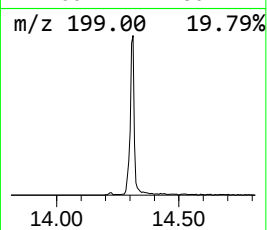
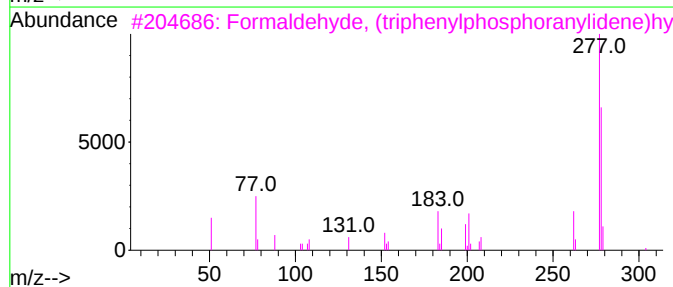
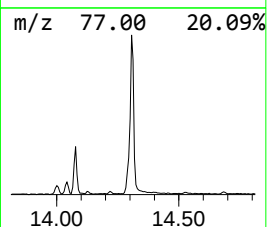
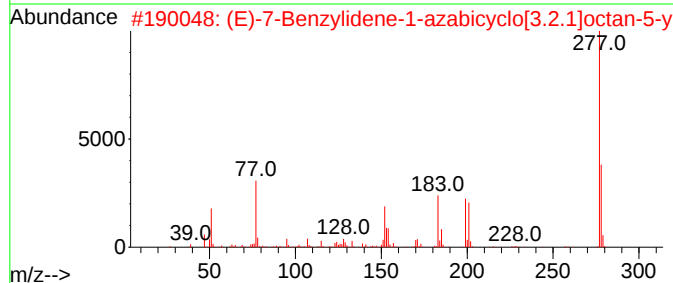
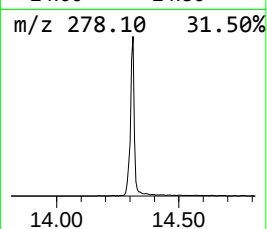
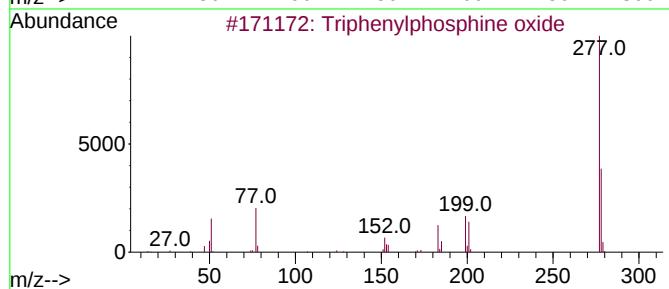
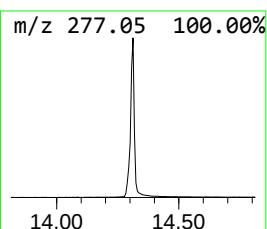
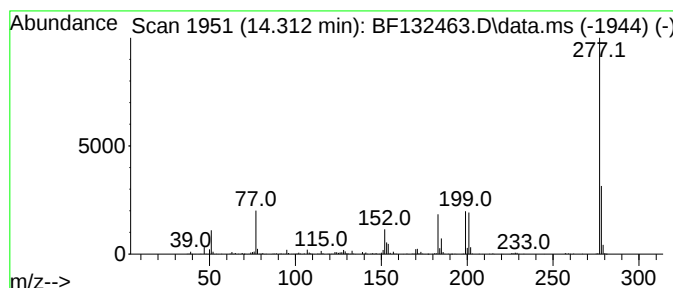
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Triphenylphosphine oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.313	11.41 ng	1125430	Chrysene-d12	14.218

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	95
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	91
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	45
4			5-Methyl-8-phenylfuro[3',2':5,6]...	277	C16H11N3O2	1000460-07-9	28
5			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021723\
Data File : BF132463.D
Acq On : 17 Feb 2023 22:16
Operator : CG\JU
Sample : 01595-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-655-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021623.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-...	5.266	33.2	ng	2505160	1	7.019	1509640	20.0
Benzophenone	10.783	24.4	ng	2745770	3	10.072	2246810	20.0
Methanone, (1-h...	11.095	3.5	ng	412058	4	11.566	2366940	20.0
n-Hexadecanoic ...	12.077	10.6	ng	1259360	4	11.566	2366940	20.0
Octadecanoic acid	12.866	3.5	ng	407931	4	11.566	2366940	20.0
Cyclotetracosane	14.048	2.0	ng	198020	5	14.218	1972570	20.0
Diethylene glyc...	14.077	2.6	ng	256480	5	14.218	1972570	20.0
Triphenylphosph...	14.313	11.4	ng	1125430	5	14.218	1972570	20.0