

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF113022\
 Data File : BF131471.D
 Acq On : 30 Nov 2022 15:02
 Operator : CG\JU
 Sample : N5793-03
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-40-SB02

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: BF131471.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.258	21	29	36	rVB	635064	840462	26.95%	3.411%
2	2.369	43	48	54	rVB	43839	53314	1.71%	0.216%
3	4.557	415	420	424	rBV	60841	68216	2.19%	0.277%
4	5.175	518	525	535	rVB	1214915	1727222	55.38%	7.010%
5	5.569	586	592	595	rBV	2261941	2289565	73.40%	9.292%
6	5.957	655	658	662	rVB	145632	116842	3.75%	0.474%
7	6.569	756	762	765	rBV	2142690	2248764	72.10%	9.126%
8	6.945	822	826	830	rVB	866563	666119	21.36%	2.703%
9	7.510	917	922	925	rBV	1674560	1684448	54.00%	6.836%
10	8.234	1041	1045	1049	rVB	965002	855745	27.44%	3.473%
11	8.628	1104	1112	1115	rBV	104821	104114	3.34%	0.423%
12	8.822	1142	1145	1150	rVB	40460	34787	1.12%	0.141%
13	9.316	1224	1229	1232	rBV	3248036	3026596	97.03%	12.283%
14	9.386	1238	1241	1245	rVB	43053	36754	1.18%	0.149%
15	9.763	1303	1305	1308	rVB	46080	37892	1.21%	0.154%
16	10.004	1341	1346	1349	rVB	1105659	1015922	32.57%	4.123%
17	10.722	1462	1468	1471	rBV	1315275	1053346	33.77%	4.275%
18	10.798	1475	1481	1484	rBV	2272566	2066060	66.24%	8.385%
19	11.028	1517	1520	1524	rBV	100732	82335	2.64%	0.334%
20	11.498	1596	1600	1604	rBV	1290709	1066235	34.18%	4.327%
21	12.022	1684	1689	1694	rBV	176489	166820	5.35%	0.677%
22	13.098	1867	1872	1875	rBV	3307970	3119132	100.00%	12.658%
23	13.992	2021	2024	2025	rBV	43394	33712	1.08%	0.137%
24	14.027	2025	2030	2046	rVB3	96089	312833	10.03%	1.270%
25	14.157	2048	2052	2055	rBV	981746	897065	28.76%	3.641%
26	14.251	2063	2068	2075	rBV	113023	131586	4.22%	0.534%
27	14.310	2075	2078	2081	rBV	45882	39077	1.25%	0.159%
28	14.616	2127	2130	2133	rBV	44688	40845	1.31%	0.166%
29	14.945	2183	2186	2191	rVB2	35546	37678	1.21%	0.153%
30	15.027	2196	2200	2206	rVB	37129	43845	1.41%	0.178%
31	15.304	2244	2247	2254	rVB	26809	36801	1.18%	0.149%
32	15.686	2307	2312	2323	rVB	523303	706528	22.65%	2.867%

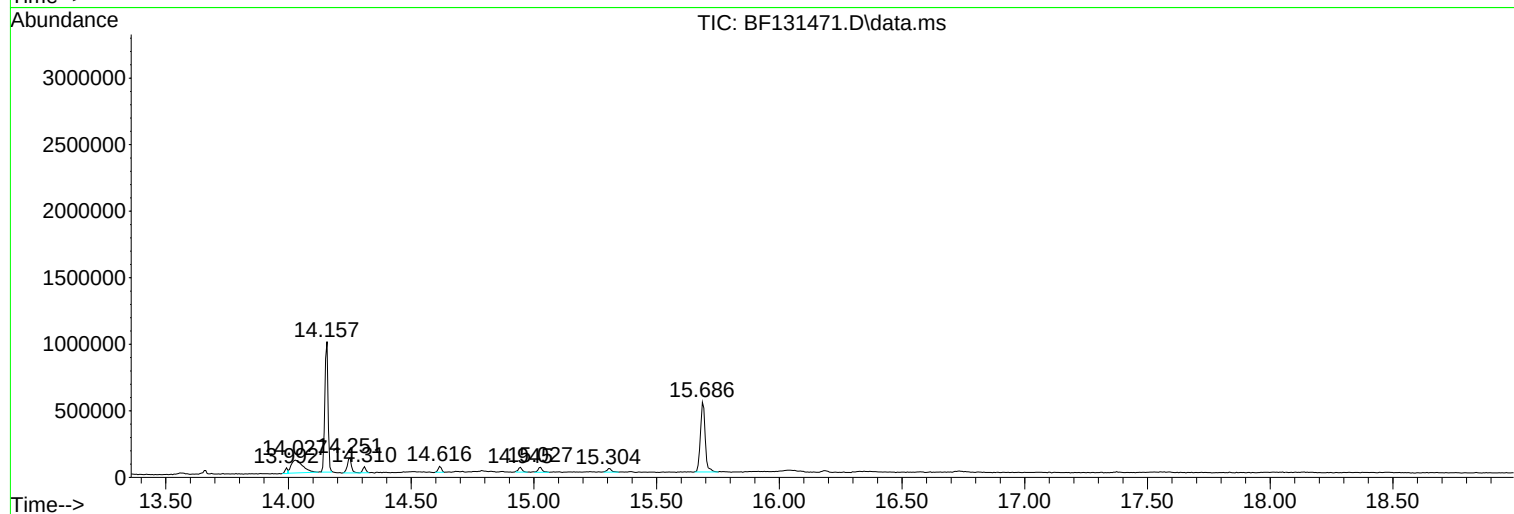
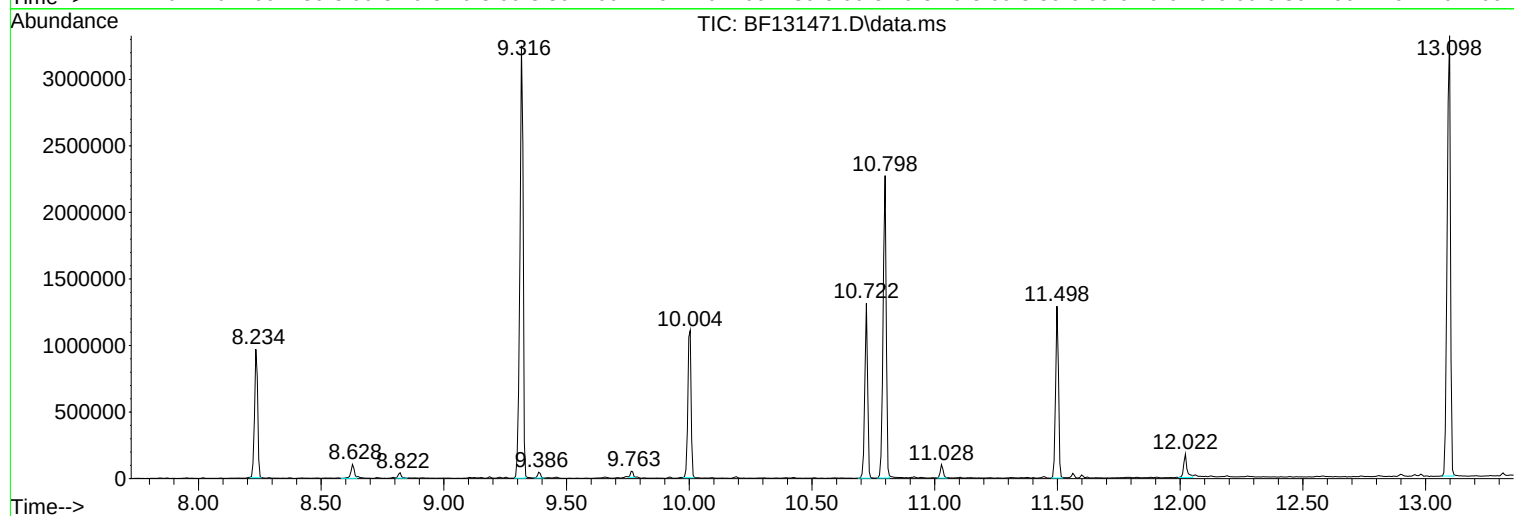
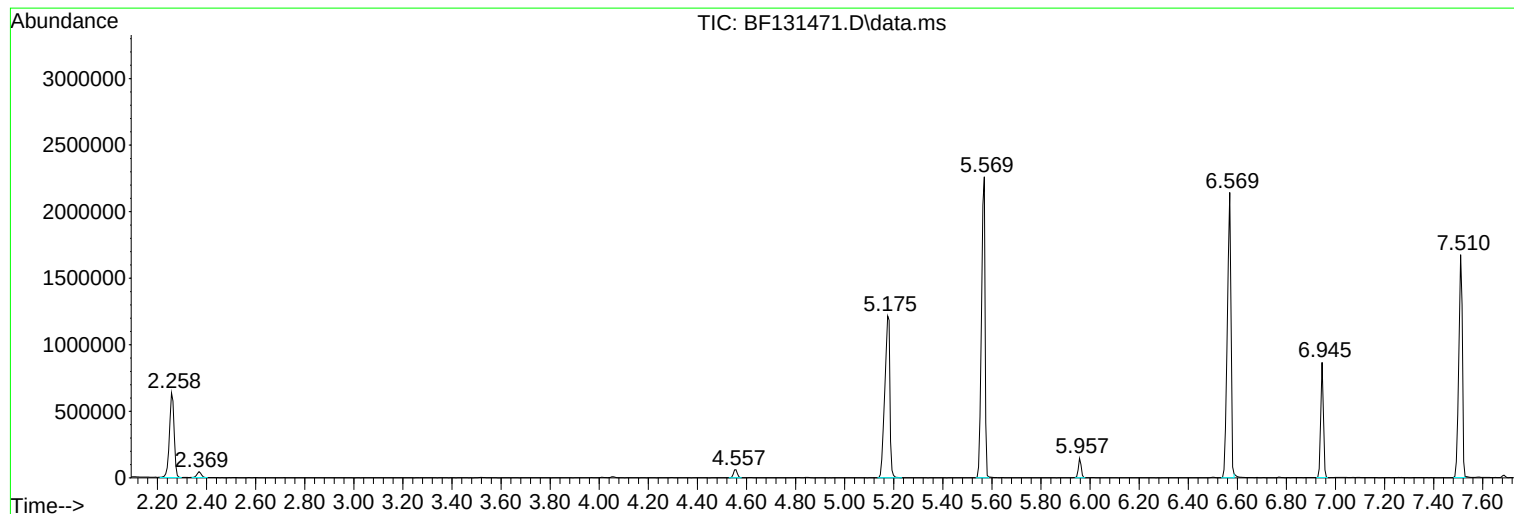
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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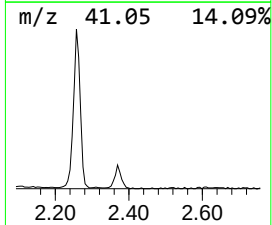
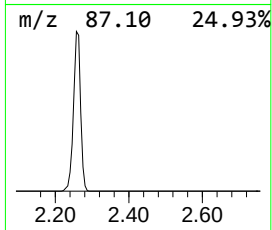
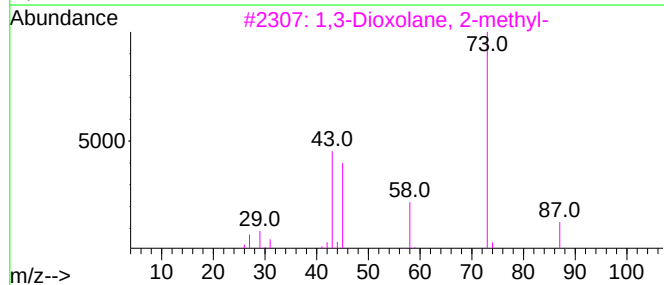
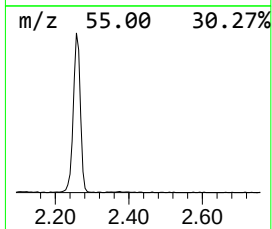
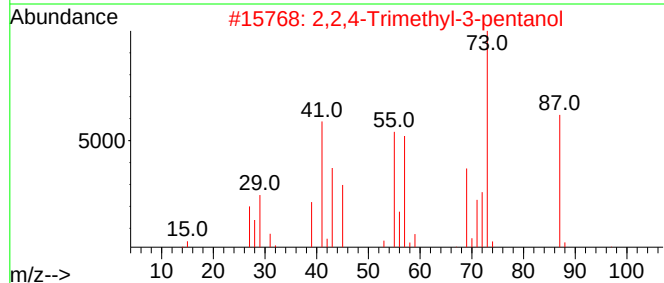
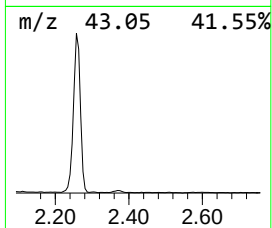
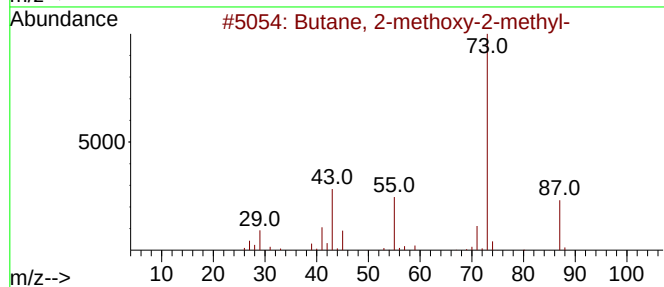
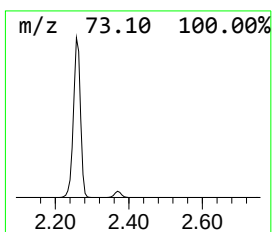
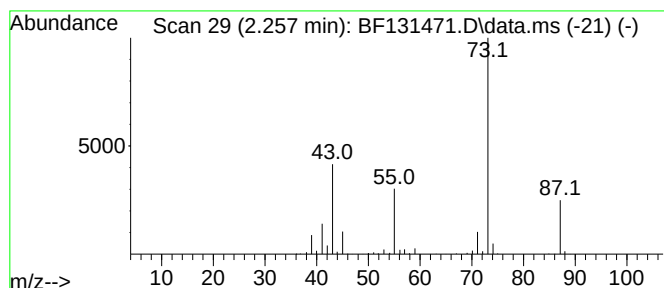
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.257	25.23 ng	840462	1,4-Dichlorobenzene-d4	6.945

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	25
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17



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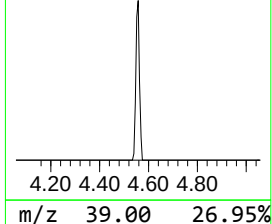
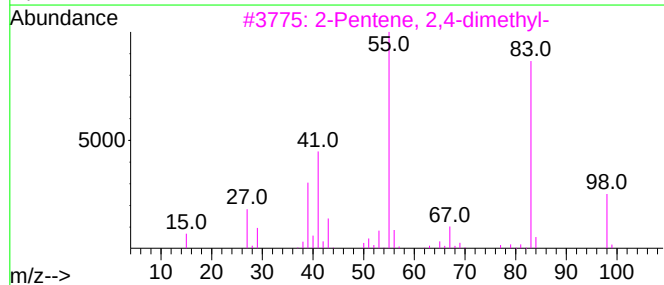
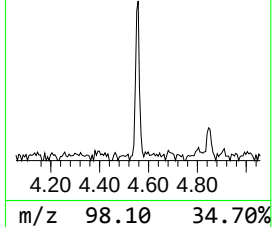
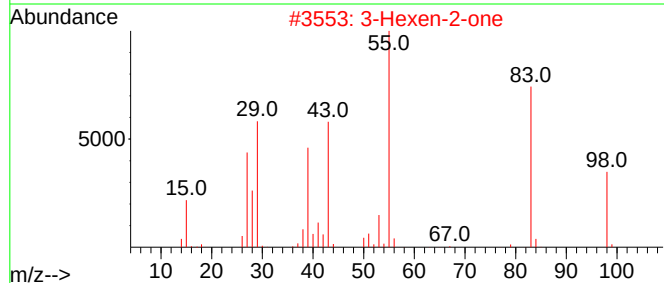
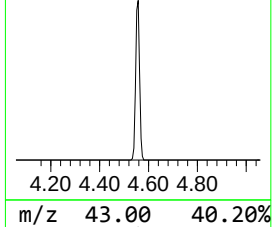
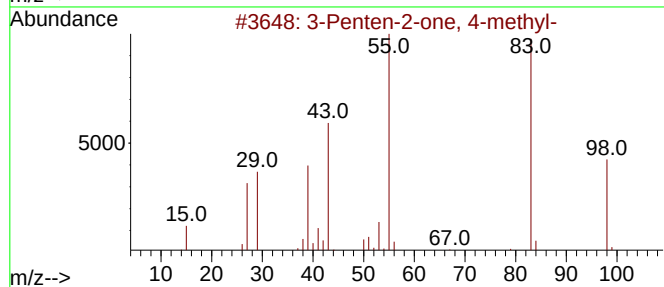
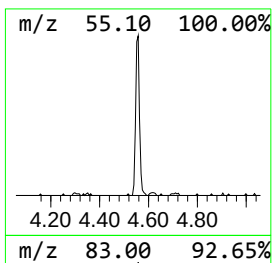
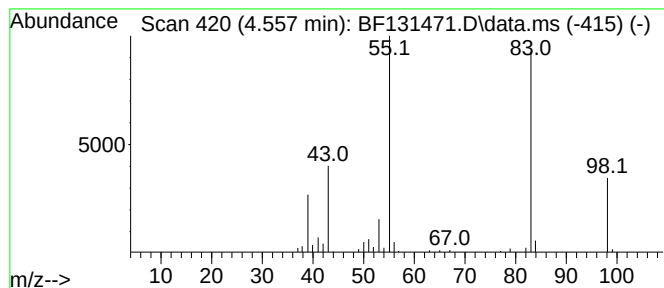
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.557	2.05 ng	68216	1,4-Dichlorobenzene-d4	6.945

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		3-Hexen-2-one	98	C6H10O	000763-93-9	91
3		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
4		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
5		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	78



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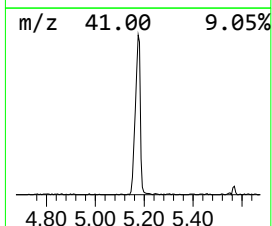
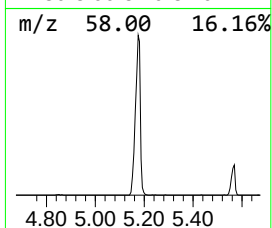
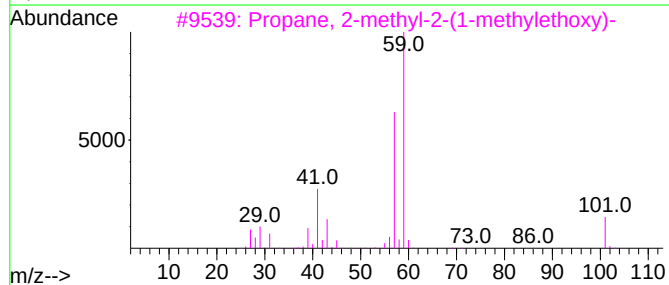
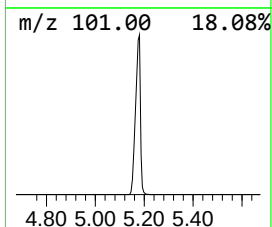
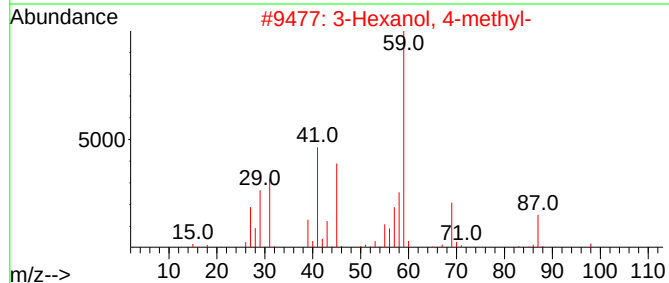
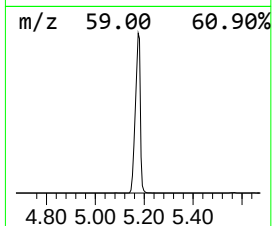
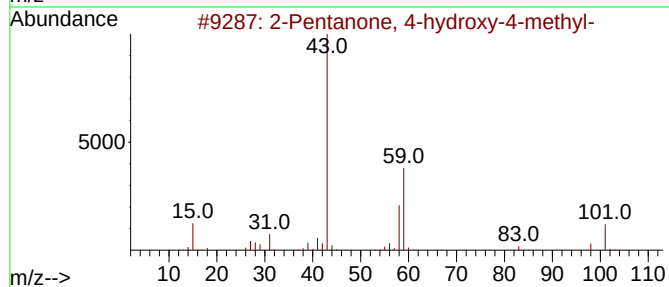
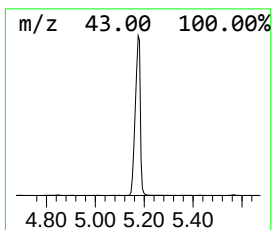
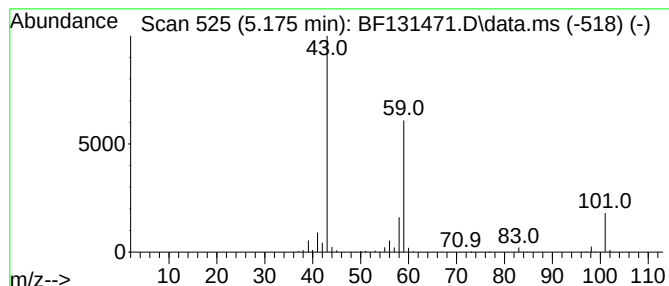
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.175	51.86 ng	1727220	1,4-Dichlorobenzene-d4	6.945

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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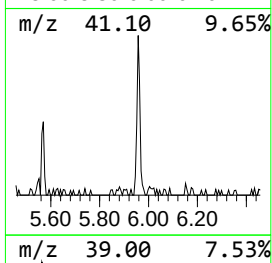
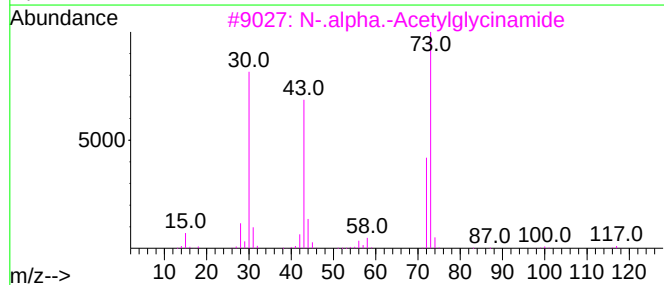
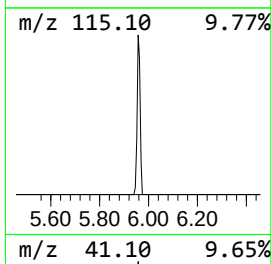
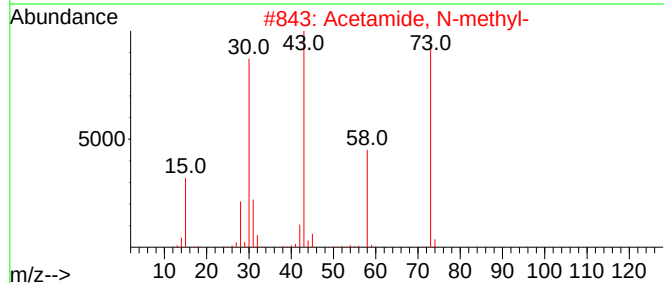
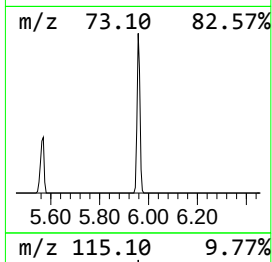
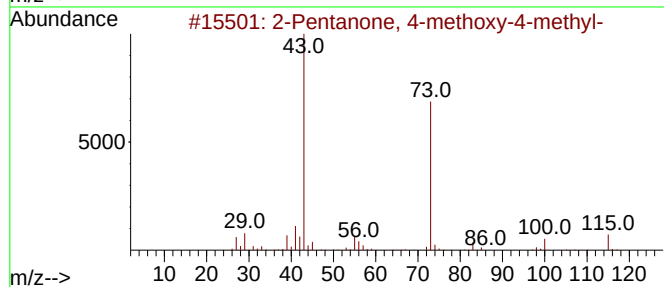
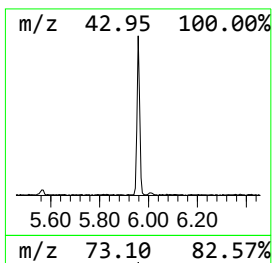
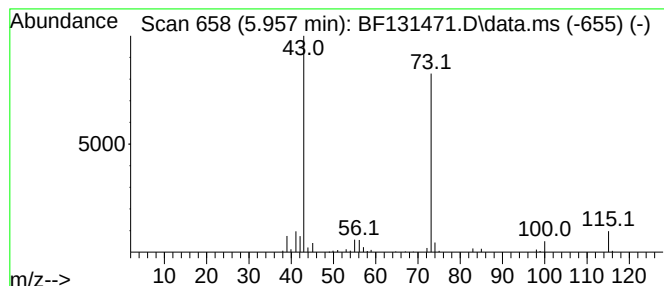
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.957	3.51 ng	116842	1,4-Dichlorobenzene-d4			6.945
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-		130	C7H14O2	000107-70-0	83
2	Acetamide, N-methyl-		73	C3H7NO	000079-16-3	47
3	N-.alpha.-Acetylglycinamide		116	C4H8N2O2	002620-63-5	38
4	N-Ethylformamide		73	C3H7NO	000627-45-2	16
5	1,3-Dioxolane, 2-propyl-		116	C6H12O2	003390-13-4	12



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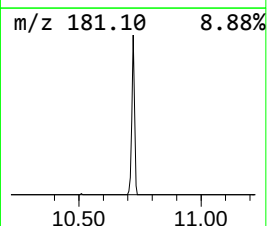
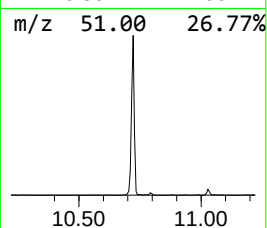
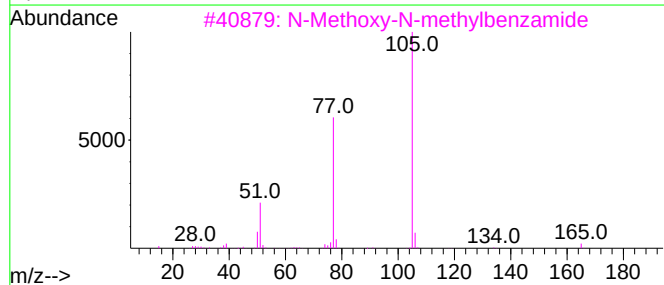
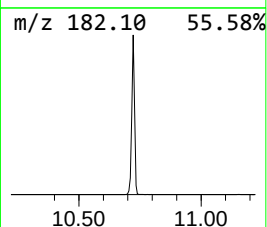
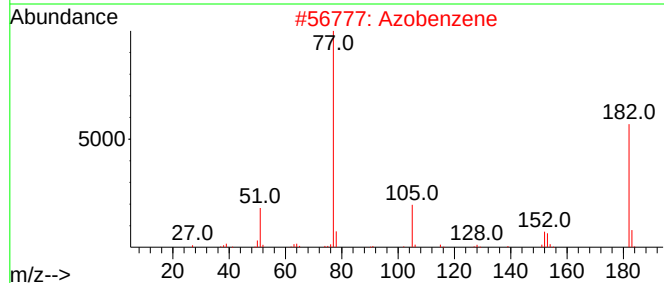
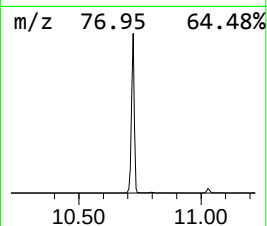
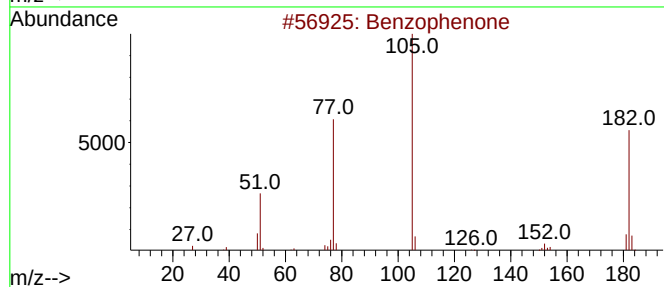
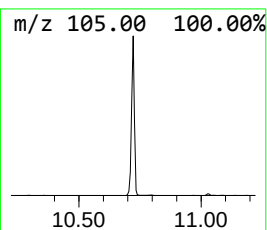
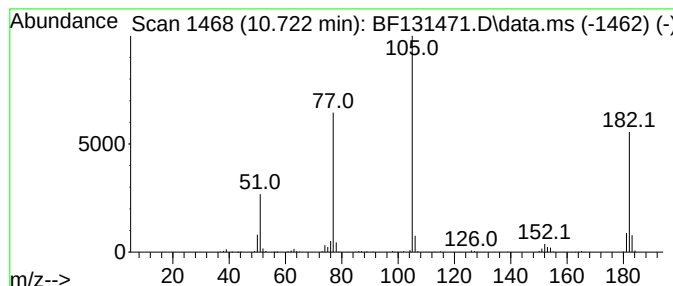
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.722	20.74 ng	1053350	Acenaphthene-d10	10.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Azobenzene	182	C12H10N2	000103-33-3	64
3			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
4			Vinyl benzoate	148	C9H8O2	000769-78-8	47
5			Benzoic acid, pentafluorophenyl ...	288	C13H5F5O2	1000360-67-9	47



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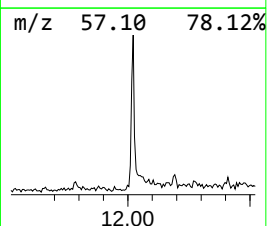
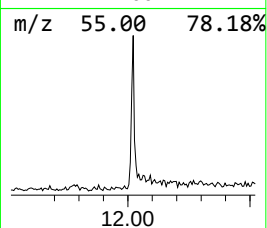
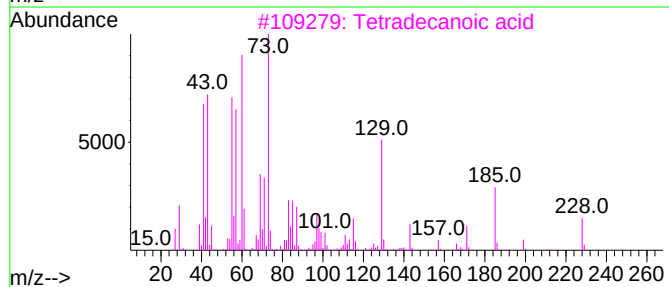
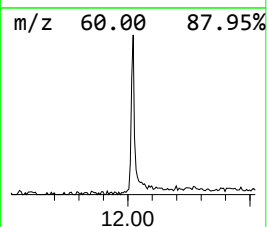
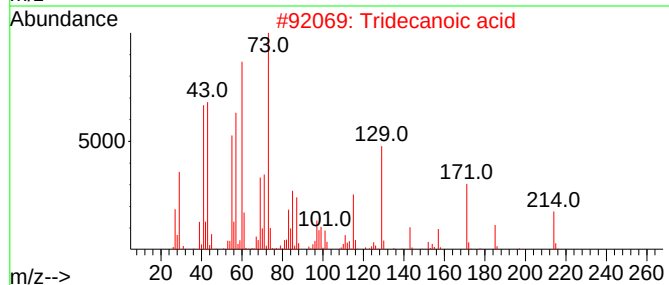
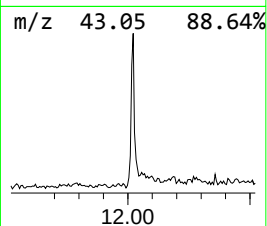
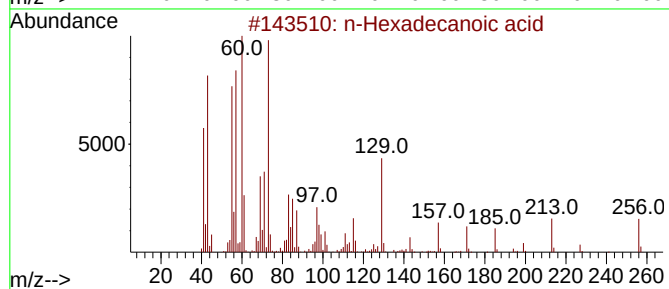
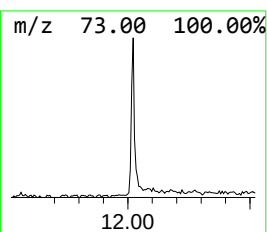
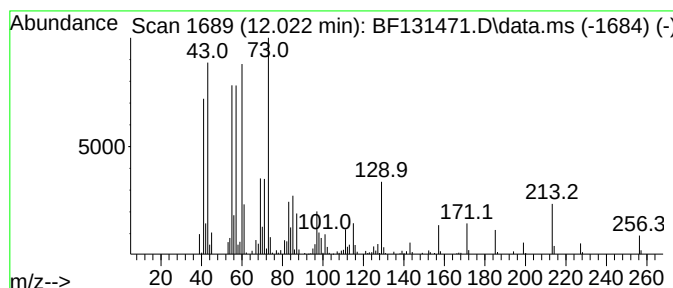
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.022	3.13 ng	166820	Phenanthrene-d10	11.498

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	96
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5			n-Decanoic acid	172	C10H20O2	000334-48-5	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF113022\
Data File : BF131471.D
Acq On : 30 Nov 2022 15:02
Operator : CG\JU
Sample : N5793-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-40-SB02

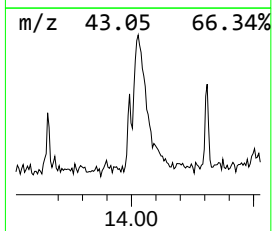
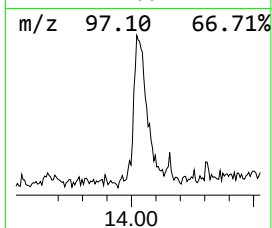
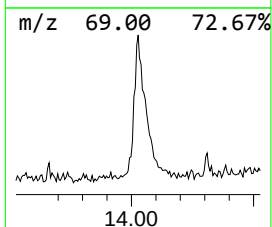
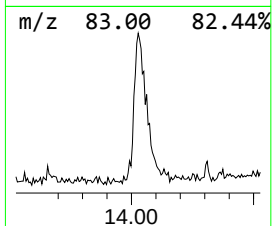
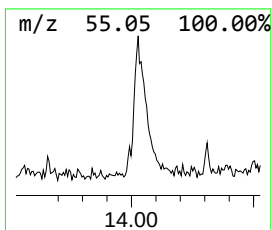
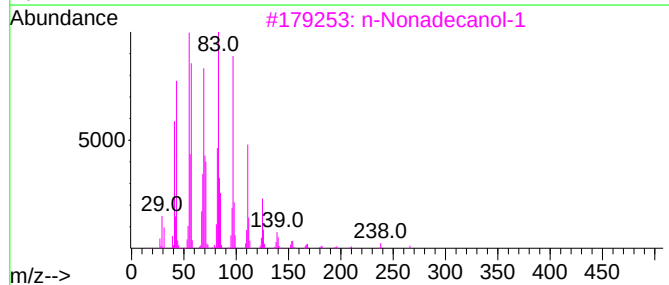
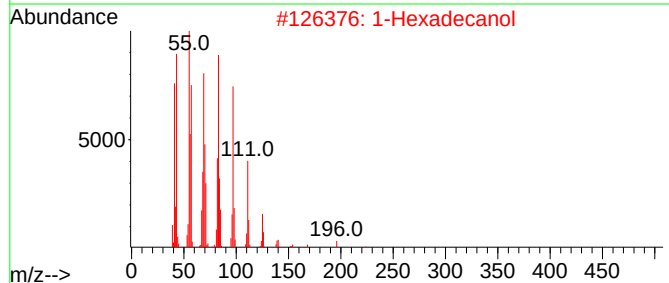
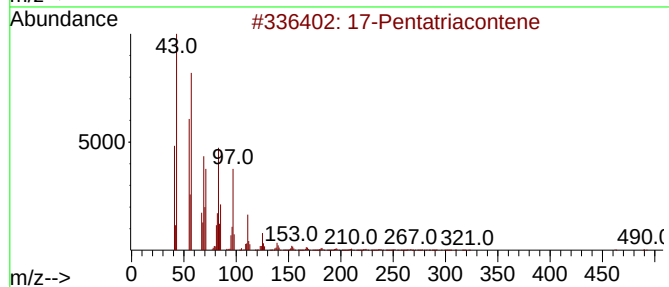
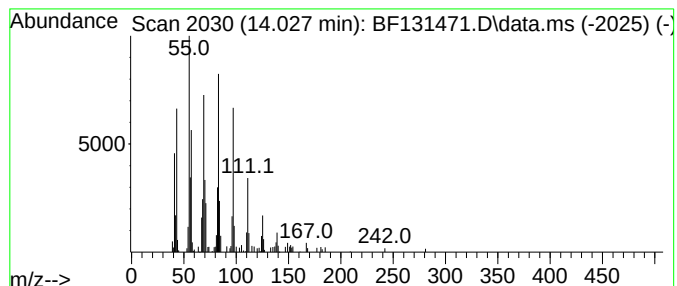
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 17-Pentatriacontene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.027	6.97 ng	312833	Chrysene-d12	14.157

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			17-Pentatriacontene	491	C35H70	006971-40-0	91
2			1-Hexadecanol	242	C16H34O	036653-82-4	90
3			n-Nonadecanol-1	284	C19H40O	001454-84-8	90
4			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	86
5			1-Octadecanol	270	C18H38O	000112-92-5	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF113022\
Data File : BF131471.D
Acq On : 30 Nov 2022 15:02
Operator : CG\JU
Sample : N5793-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-40-SB02

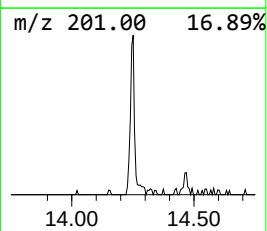
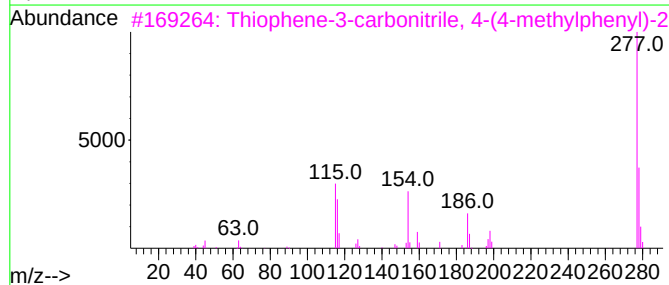
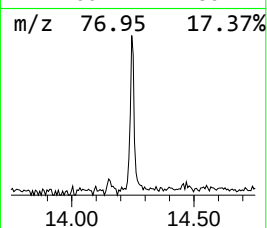
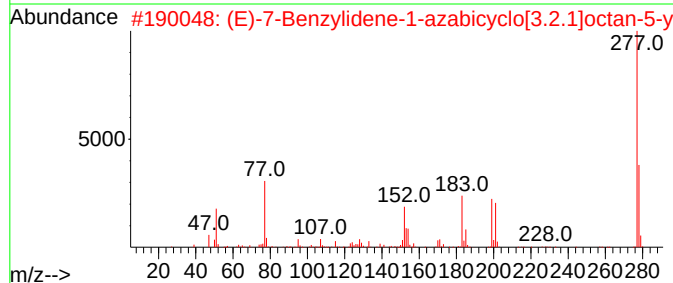
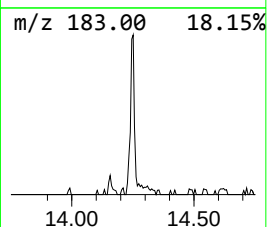
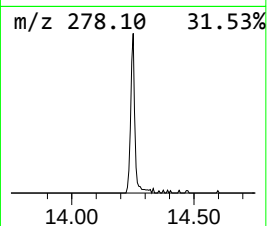
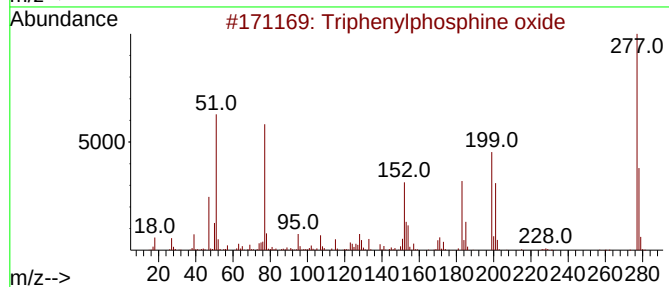
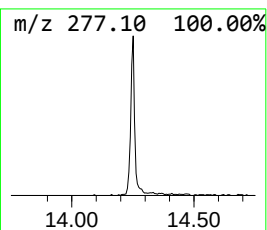
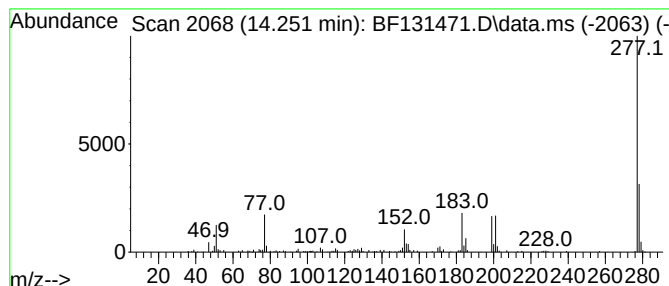
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Triphenylphosphine oxide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.251	2.93 ng	131586	Chrysene-d12	14.157

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	90
3			Thiophene-3-carbonitrile, 4-(4-m...	277	C13H11NO2S2	1000268-75-0	38
4			Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	33
5			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	28



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF113022\
Data File : BF131471.D
Acq On : 30 Nov 2022 15:02
Operator : CG\JU
Sample : N5793-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-40-SB02

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

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.257	25.2	ng	840462	1	6.945	666119	20.0
3-Penten-2-one,...	4.557	2.0	ng	68216	1	6.945	666119	20.0
2-Pentanone, 4-...	5.175	51.9	ng	1727220	1	6.945	666119	20.0
2-Pentanone, 4-...	5.957	3.5	ng	116842	1	6.945	666119	20.0
Benzophenone	10.722	20.7	ng	1053350	3	10.004	1015920	20.0
n-Hexadecanoic ...	12.022	3.1	ng	166820	4	11.498	1066240	20.0
17-Pentatriacon...	14.027	7.0	ng	312833	5	14.157	897065	20.0
Triphenylphosph...	14.251	2.9	ng	131586	5	14.157	897065	20.0