

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112822\
 Data File : BF131424.D
 Acq On : 28 Nov 2022 11:55
 Operator : CG\JU
 Sample : N5766-02
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CR-2

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: BF131424.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.263	21	30	36	rBV	670465	895716	42.11%	5.846%
2	5.175	520	525	532	rVB	398929	468300	22.02%	3.057%
3	5.563	586	591	594	rBV	1893959	1765262	82.99%	11.522%
4	6.569	756	762	765	rBV	1786305	1765580	83.00%	11.524%
5	6.951	823	827	830	rVB	615197	488508	22.97%	3.189%
6	7.516	918	923	926	rBV	1295861	1153104	54.21%	7.527%
7	8.239	1042	1046	1049	rBV	789067	625209	29.39%	4.081%
8	9.322	1224	1230	1233	rBV	2506287	2127118	100.00%	13.884%
9	10.004	1342	1346	1349	rBV	900889	727362	34.19%	4.748%
10	10.798	1476	1481	1484	rBV	1614443	1359865	63.93%	8.876%
11	11.504	1597	1601	1604	rBV	817923	724216	34.05%	4.727%
12	13.098	1868	1872	1875	rBV	2306870	1998479	93.95%	13.044%
13	13.998	2021	2025	2042	rBV	92753	177423	8.34%	1.158%
14	14.157	2049	2052	2056	rBV	523844	464849	21.85%	3.034%
15	14.257	2063	2069	2076	rBV	49124	56557	2.66%	0.369%
16	14.951	2181	2187	2192	rBV2	19788	33368	1.57%	0.218%
17	15.698	2308	2314	2319	rBV	310770	404028	18.99%	2.637%
18	18.809	2834	2843	2856	rBV	19762	85642	4.03%	0.559%

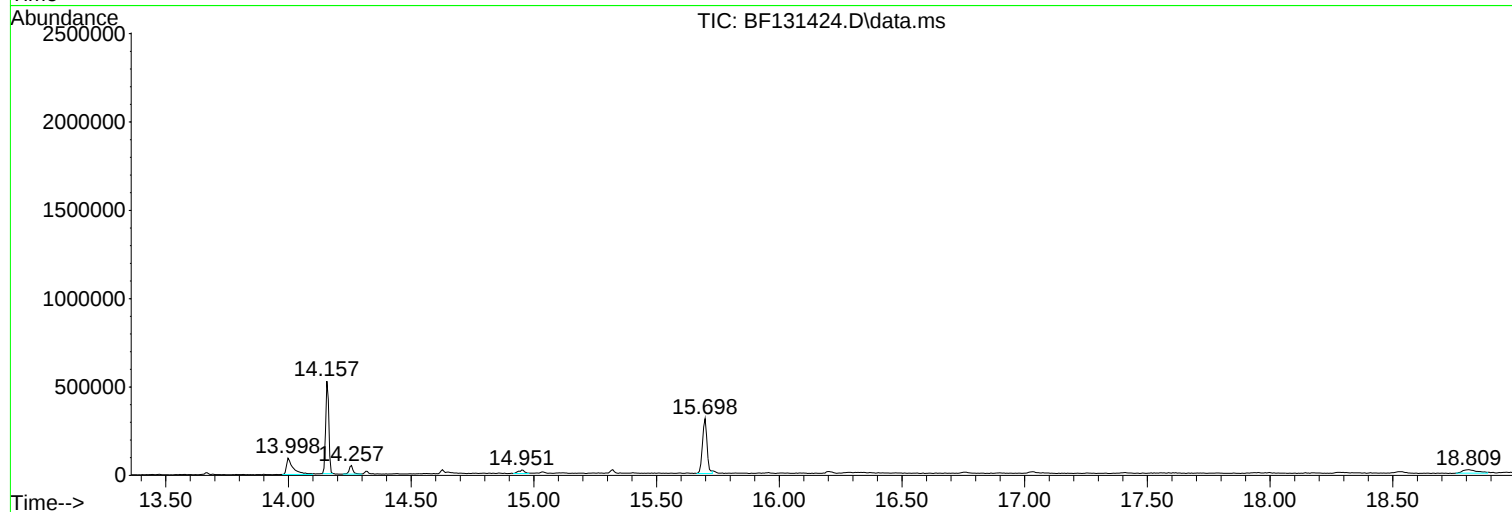
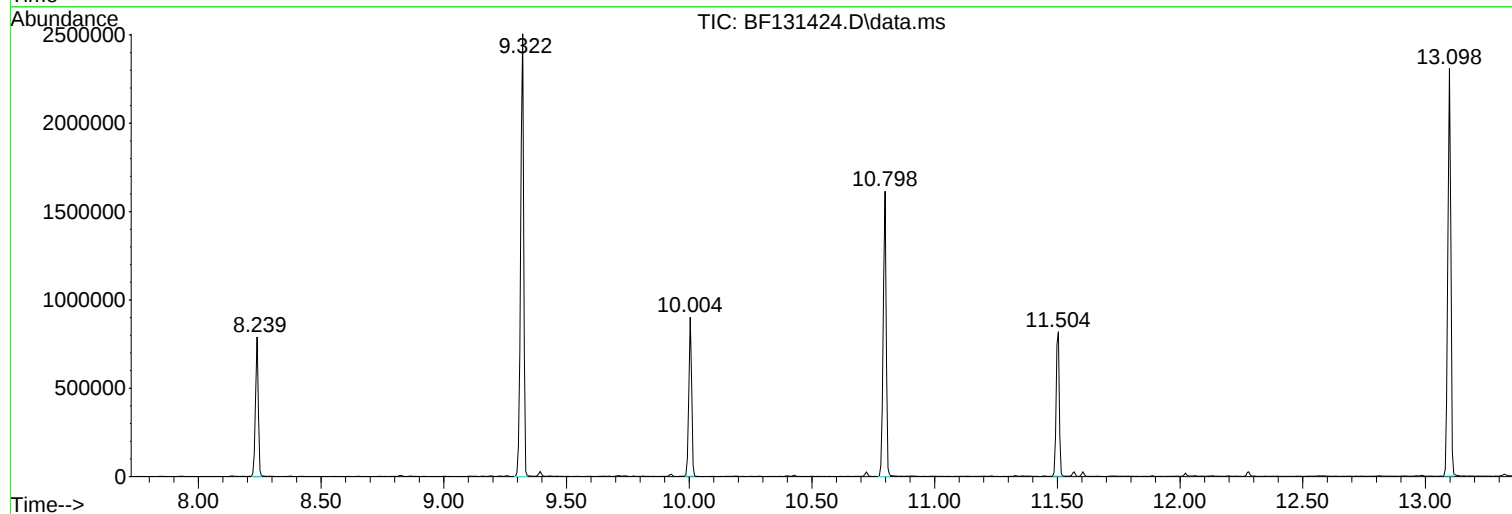
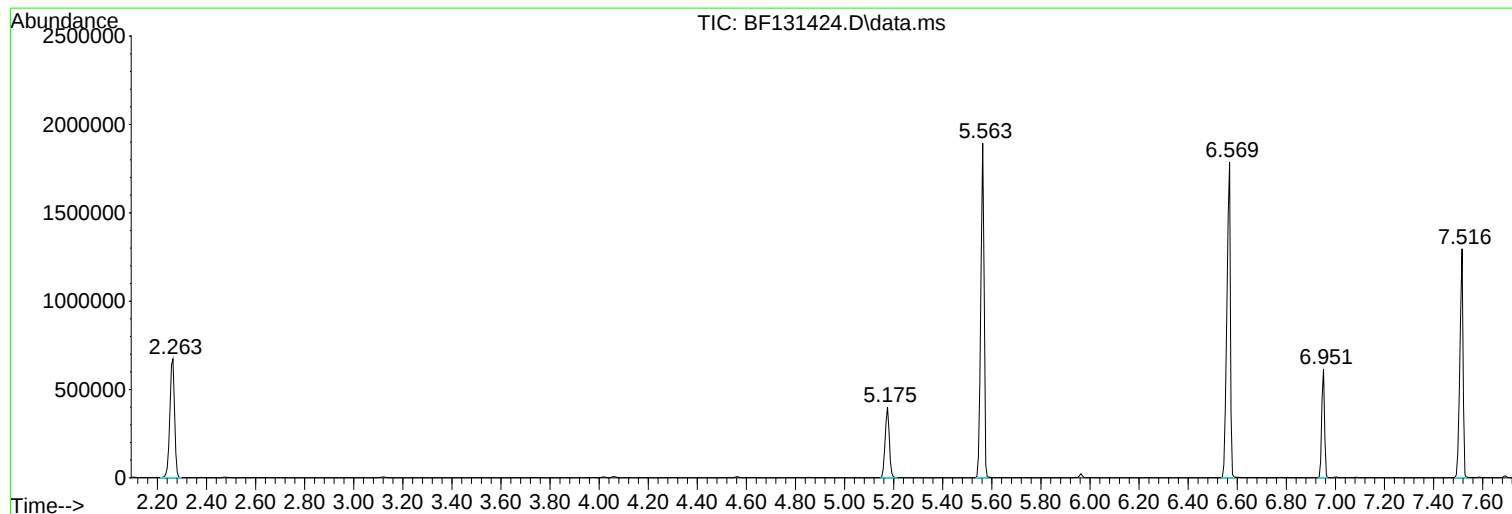
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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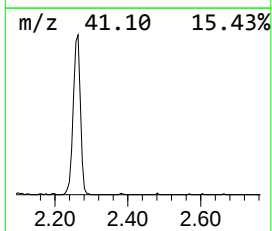
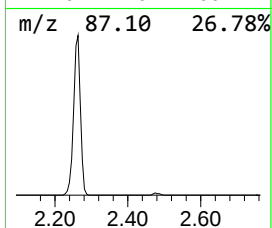
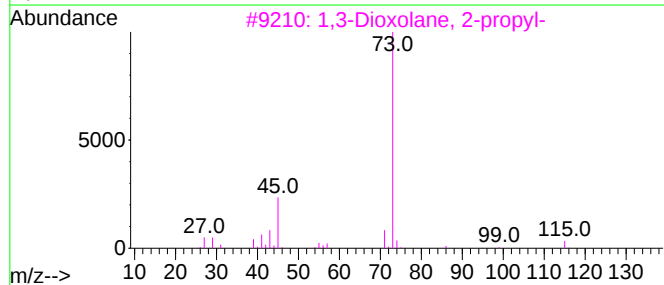
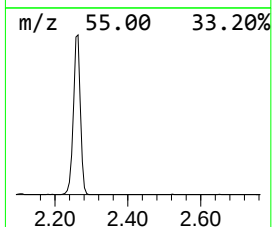
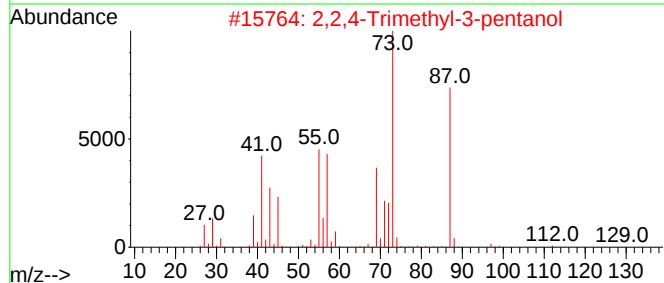
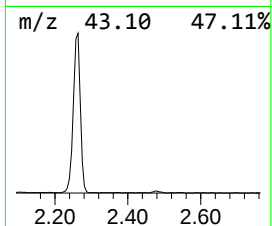
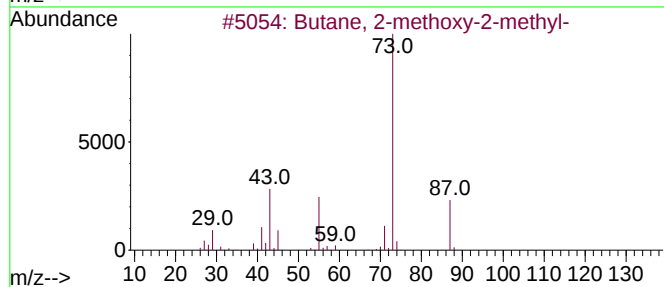
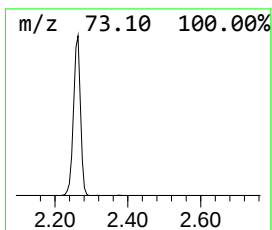
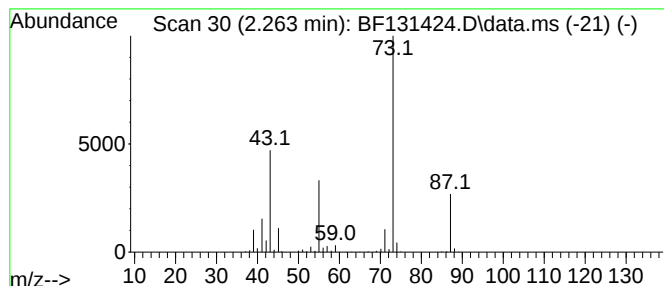
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.263	36.67 ng	895716	1,4-Dichlorobenzene-d4	6.951

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	40
3			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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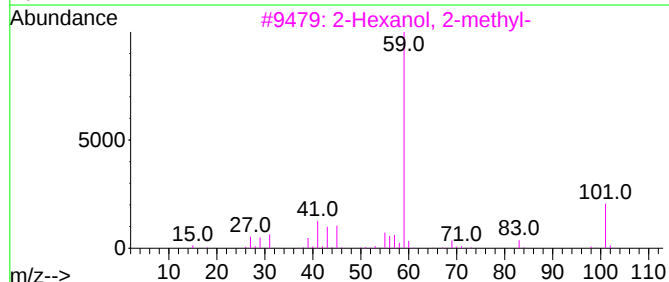
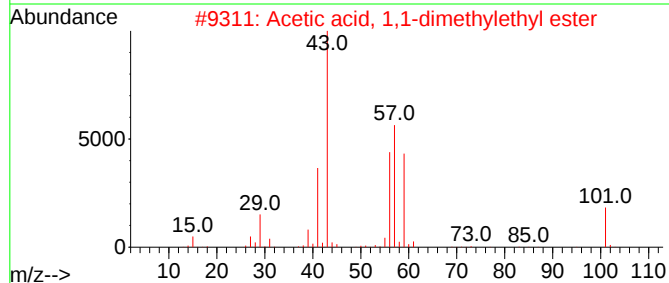
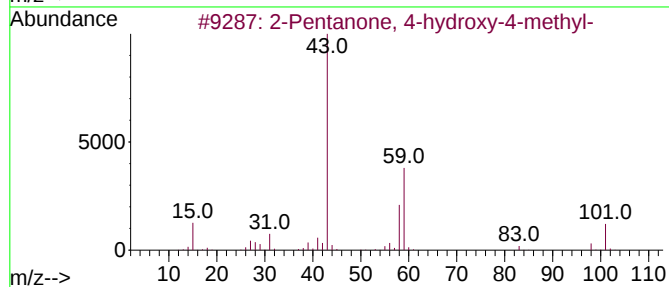
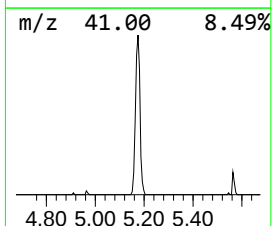
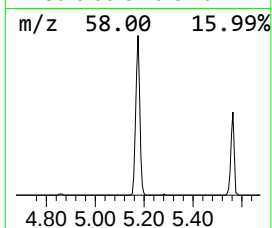
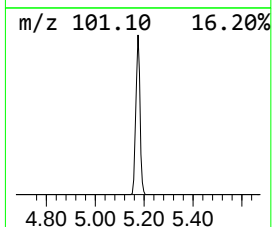
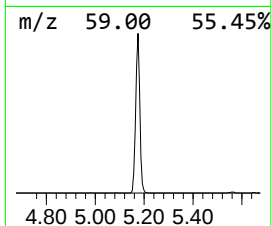
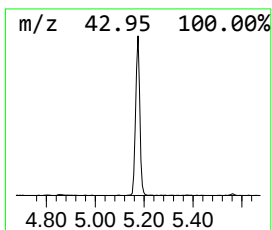
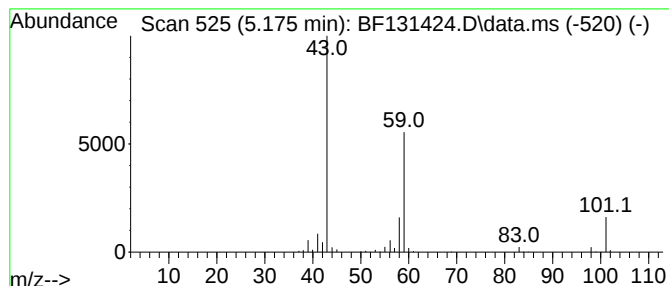
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.175	19.17 ng	468300	1,4-Dichlorobenzene-d4	6.951

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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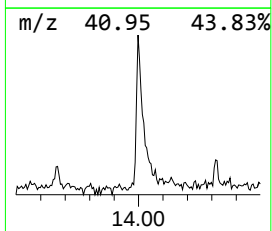
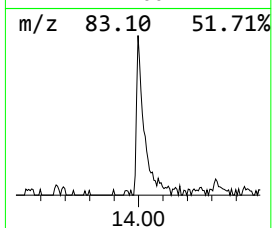
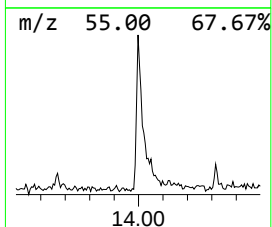
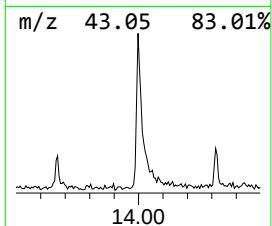
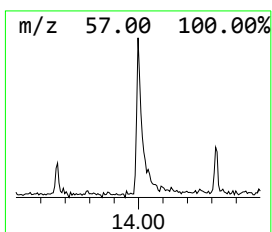
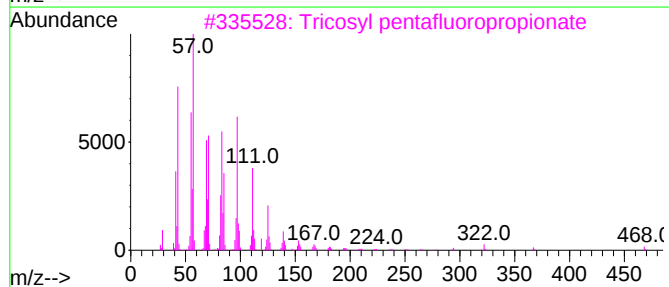
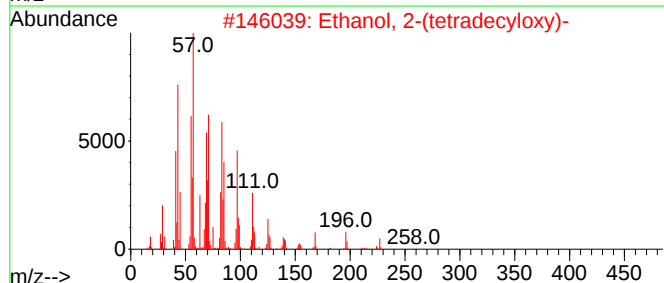
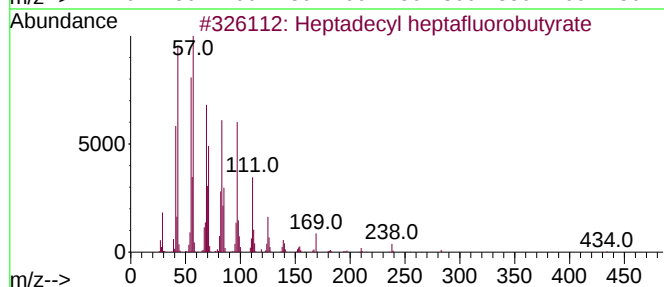
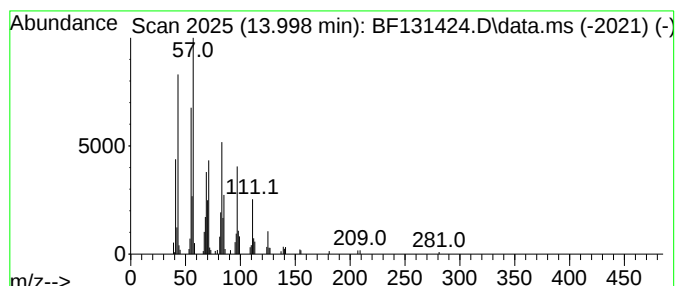
Instrument :
BNA_F
ClientSampleId :
CR-2

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

Peak Number 3 Heptadecyl heptafluorobutyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.998	7.63 ng	177423	Chrysene-d12		14.157	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate		452	C21H35F7O2	959085-66-6	91
2	Ethanol, 2-(tetradecyloxy)-		258	C16H34O2	002136-70-1	91
3	Tricosyl pentafluoropropionate		486	C26H47F5O2	1000351-81-0	91
4	Tricosyl trifluoroacetate		436	C25H47F3O2	1000351-75-1	91
5	Tetracosyl heptafluorobutyrate		550	C28H49F7O2	1000351-83-7	91



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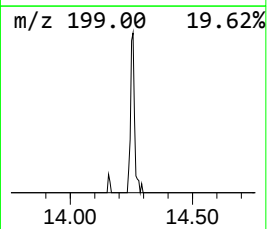
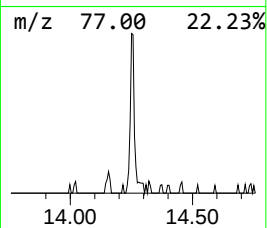
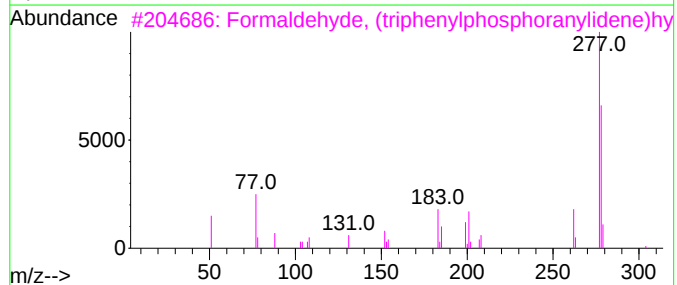
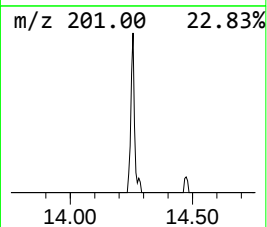
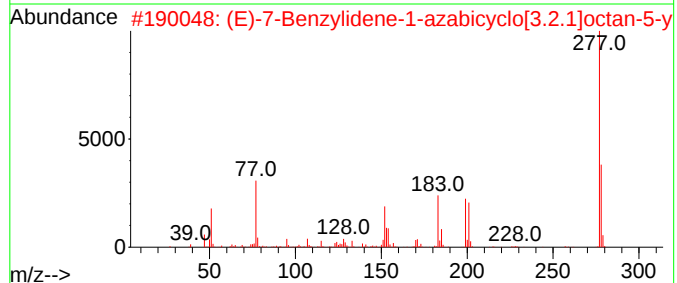
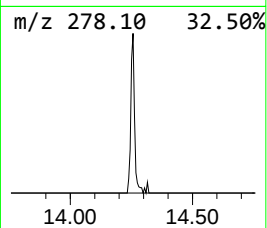
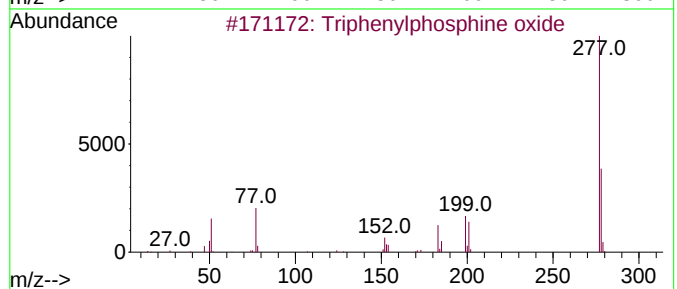
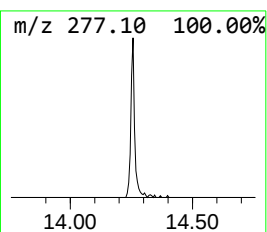
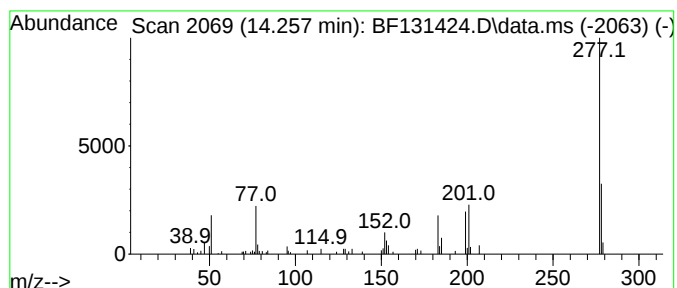
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Peak Number 4 Triphenylphosphine oxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.257	2.43 ng	56557	Chrysene-d12	14.157

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	94
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	47
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	45
4			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	25
5			1H-Indole-3-acetic acid, 5-[(tri...	277	C14H19N03Si	072101-35-0	25



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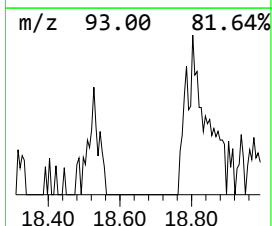
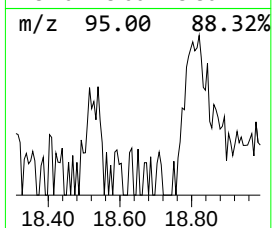
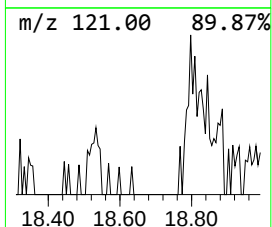
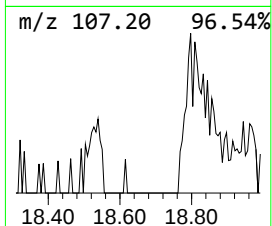
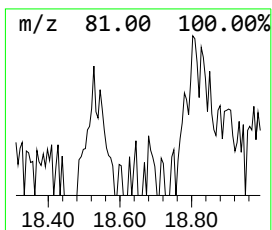
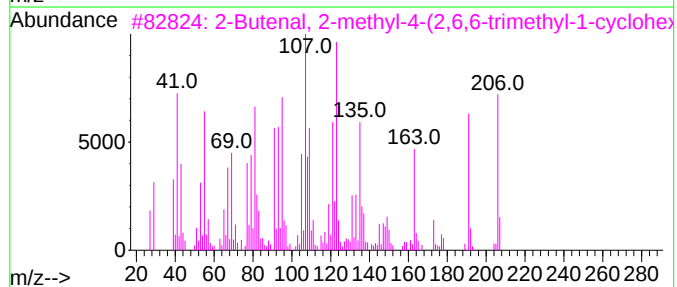
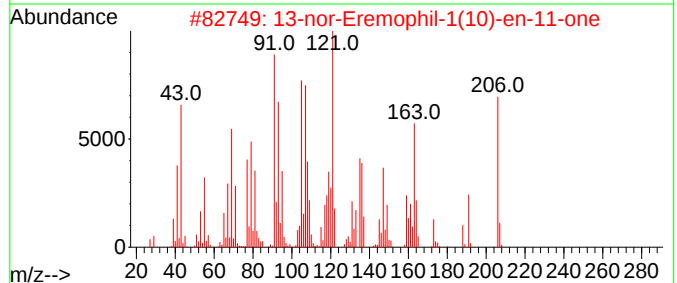
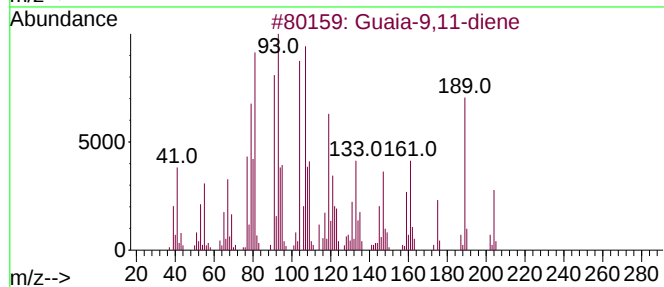
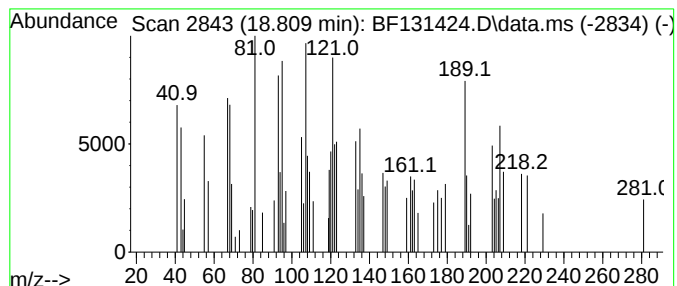
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Guaia-9,11-diene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.809	4.24 ng	85642	Perylene-d12	15.698

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Guaia-9,11-diene	204	C15H24	1000374-19-8	74
2			13-nor-Eremophil-1(10)-en-11-one	206	C14H22O	054275-21-7	42
3			2-Butenal, 2-methyl-4-(2,6,6-trimethyl-1-cyclohexyl)-	206	C14H22O	003155-71-3	41
4			1,5-Cyclododecadiene, 1,5-dimethyl-	204	C15H24	015423-57-1	41
5			2,12-Dimethylidenecyclododecan-1-one	206	C14H22O	069915-61-3	38



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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...	2.263	36.7	ng	895716	1	6.951	488508	20.0
2-Pentanone, 4-...	5.175	19.2	ng	468300	1	6.951	488508	20.0
Heptadecyl hept...	13.998	7.6	ng	177423	5	14.157	464849	20.0
Triphenylphosph...	14.257	2.4	ng	56557	5	14.157	464849	20.0
Guaia-9,11-diene	18.809	4.2	ng	85642	6	15.698	404028	20.0