

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121622\
 Data File : BF131671.D
 Acq On : 16 Dec 2022 17:38
 Operator : CG\JU
 Sample : N6037-06
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RB-20-(7-9)

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-BF120822.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131671.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.128	3	7	13	rVB	302655	382707	19.40%	3.005%
2	5.087	505	510	516	rVB	178499	215889	10.94%	1.695%
3	5.493	574	579	582	rBV	1751507	1558193	78.98%	12.235%
4	6.510	747	752	755	rBV	1676113	1566504	79.40%	12.300%
5	6.881	811	815	818	rBV	477540	400903	20.32%	3.148%
6	7.445	906	911	914	rBV	1141359	989604	50.16%	7.770%
7	8.169	1030	1034	1037	rBV	624012	493853	25.03%	3.878%
8	9.251	1213	1218	1221	rBV	2020400	1802158	91.34%	14.150%
9	9.933	1330	1334	1337	rBV	701610	563740	28.57%	4.426%
10	10.651	1452	1456	1459	rBV	102297	81950	4.15%	0.643%
11	10.727	1464	1469	1472	rBV	1260913	1136824	57.62%	8.926%
12	11.427	1584	1588	1591	rBV	753139	598514	30.34%	4.699%
13	13.021	1854	1859	1862	rBV	2376883	1972994	100.00%	15.492%
14	13.933	2008	2014	2015	rBV3	26694	46032	2.33%	0.361%
15	14.080	2035	2039	2042	rVB	489443	447382	22.68%	3.513%
16	14.174	2051	2055	2061	rVB	28475	30164	1.53%	0.237%
17	14.939	2180	2185	2188	rBV	54235	57245	2.90%	0.449%
18	15.580	2289	2294	2302	rBV2	313299	391241	19.83%	3.072%

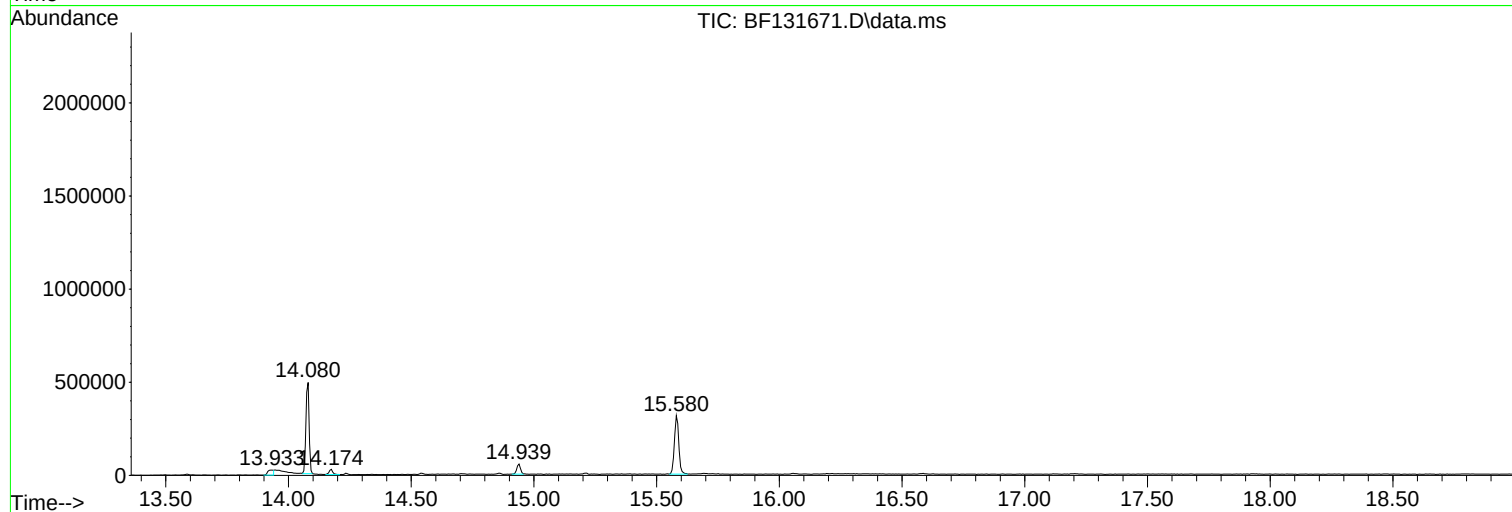
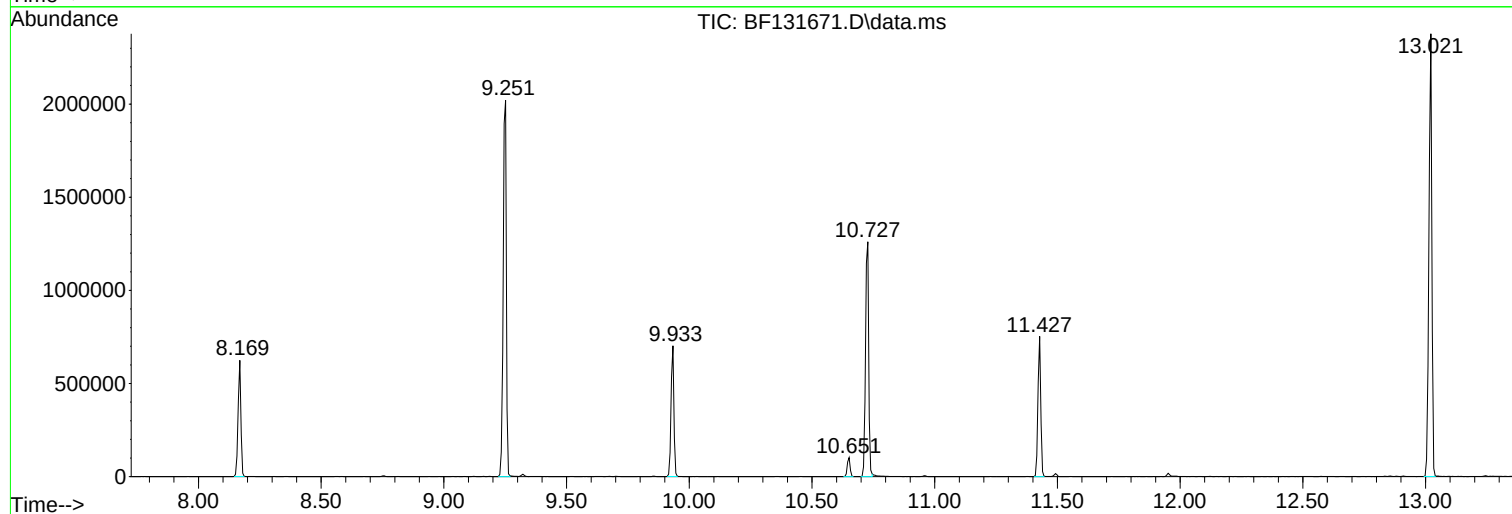
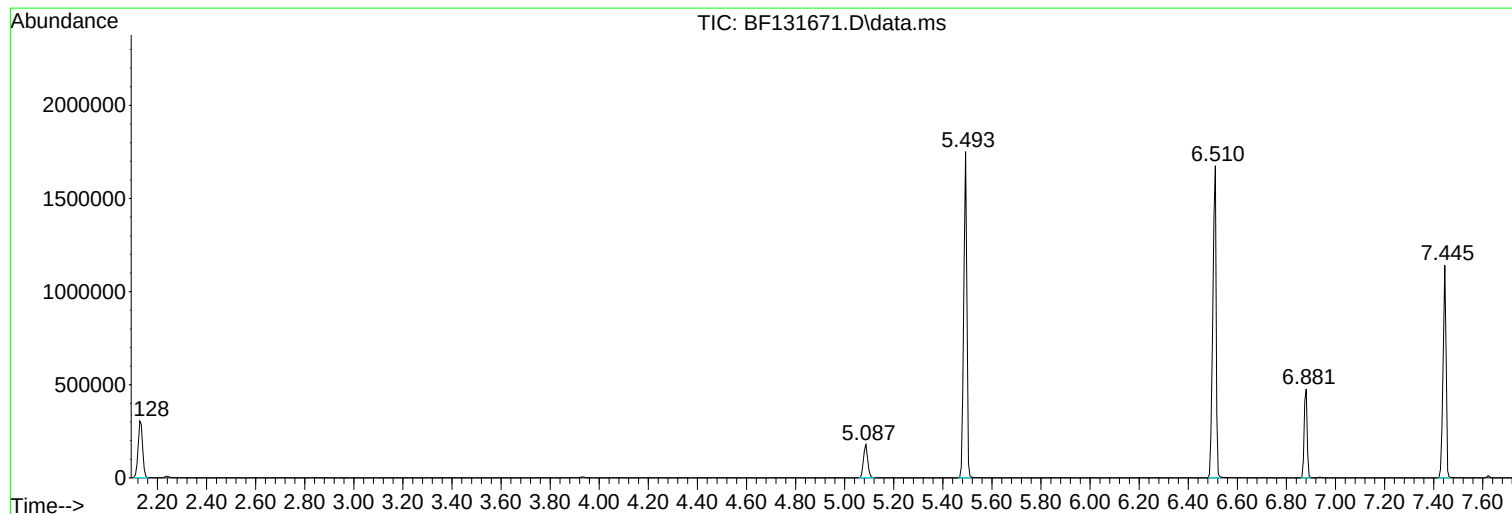
Sum of corrected areas: 12735897

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.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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Instrument :
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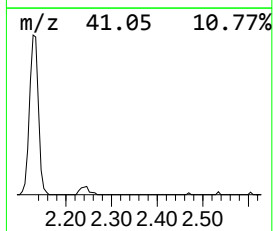
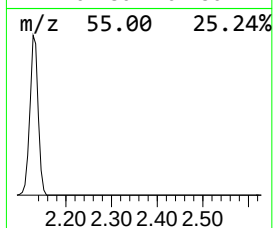
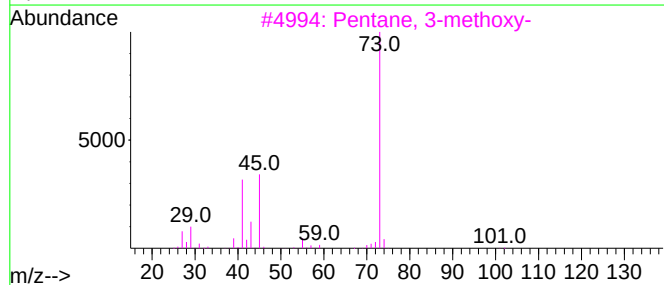
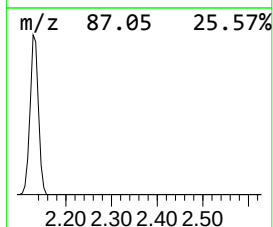
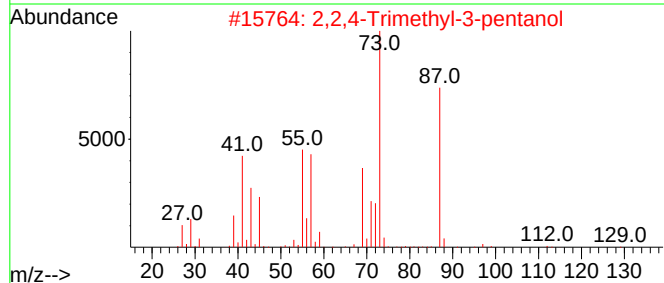
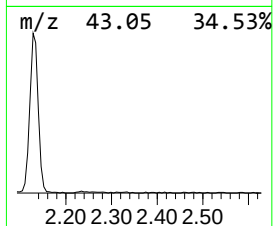
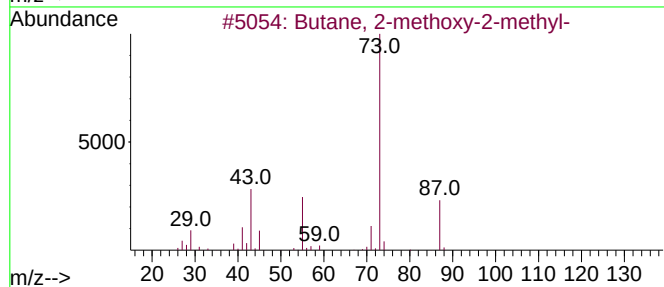
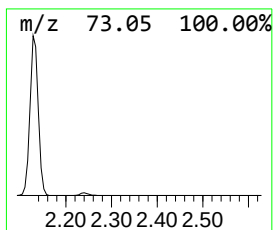
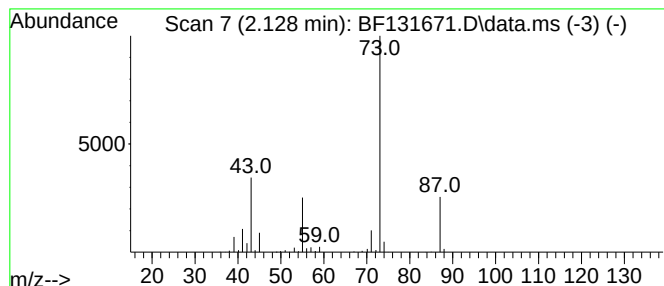
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.128	19.09 ng	382707	1,4-Dichlorobenzene-d4	6.881

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	10
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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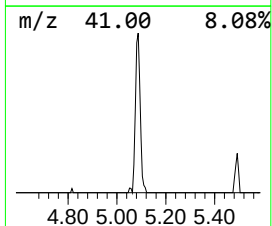
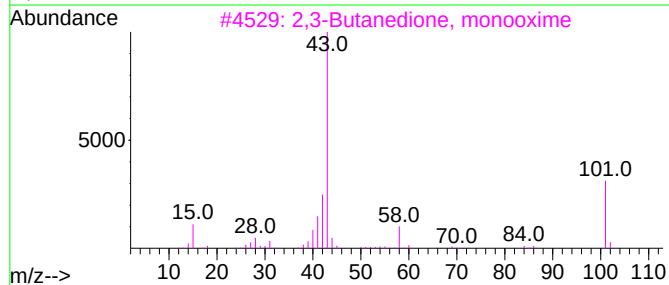
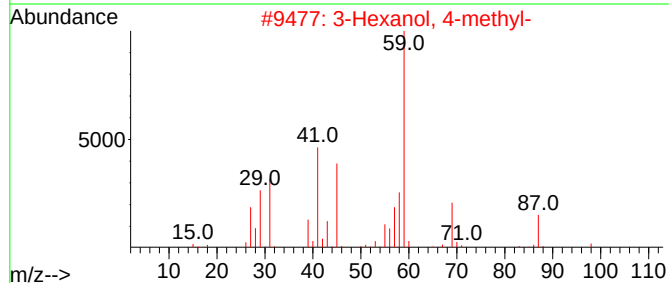
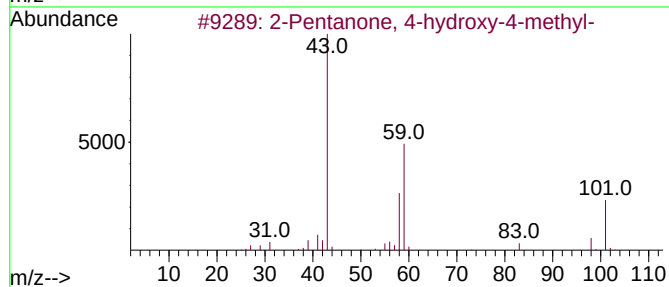
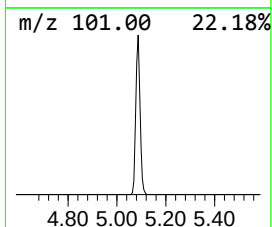
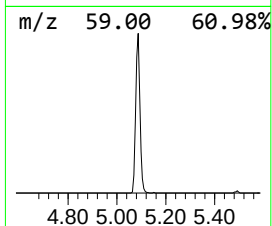
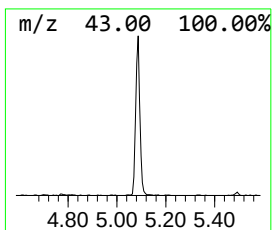
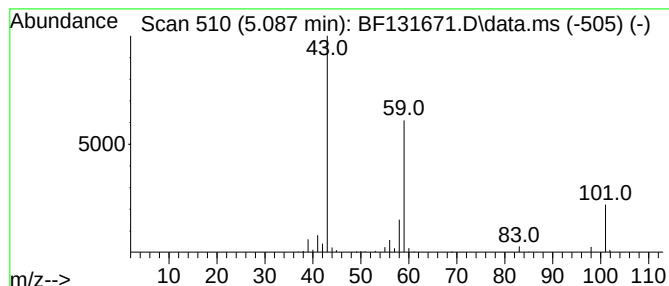
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.087	10.77 ng	215889	1,4-Dichlorobenzene-d4	6.881

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5			Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	17



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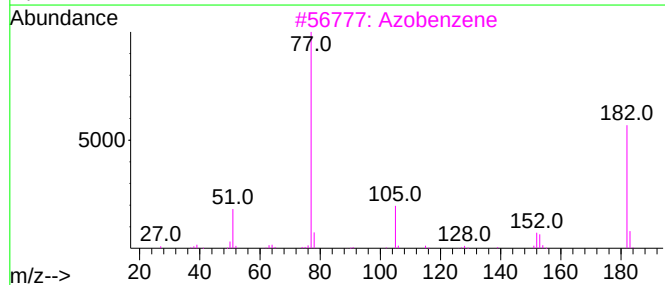
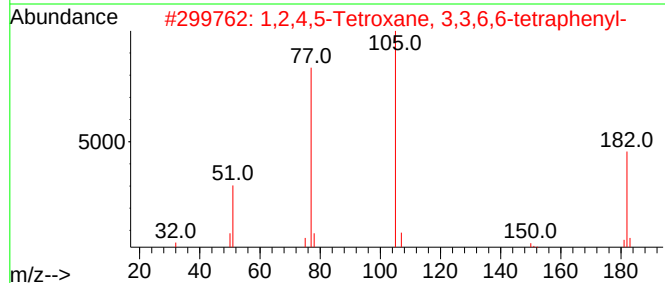
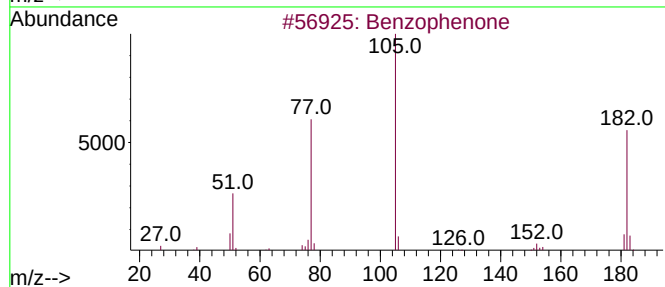
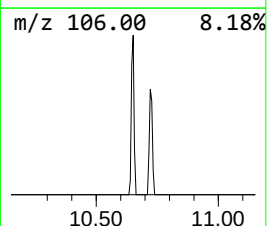
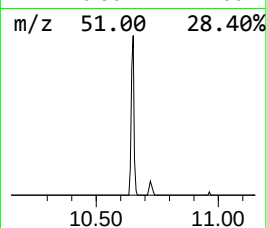
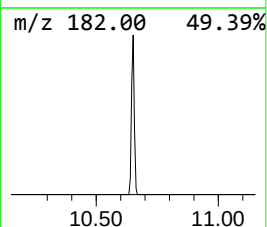
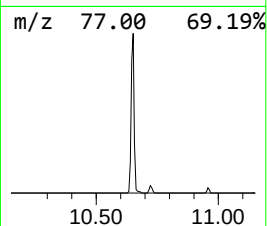
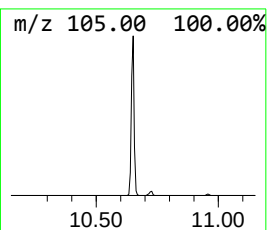
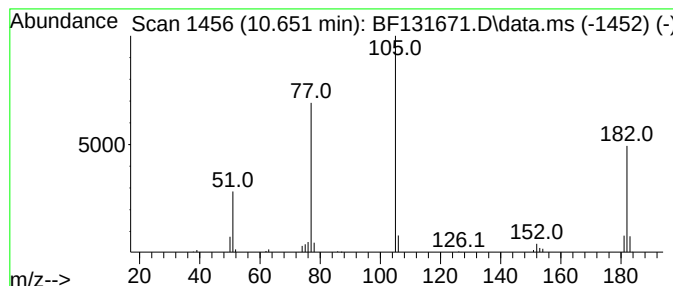
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.651	2.91 ng	81950	Acenaphthene-d10	9.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	78
3			Azobenzene	182	C12H10N2	000103-33-3	59
4			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	52
5			Benzoyl bromide	184	C7H5BrO	000618-32-6	47



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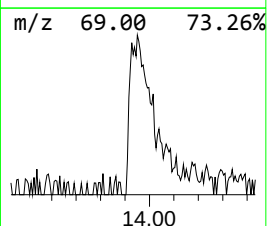
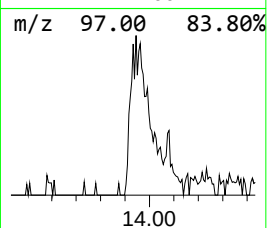
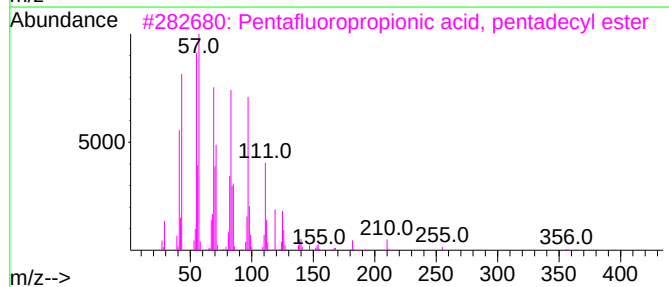
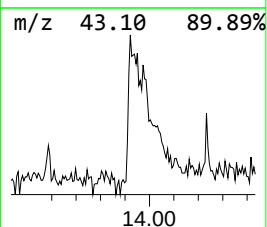
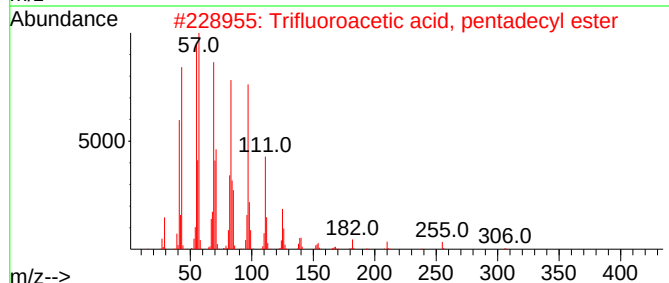
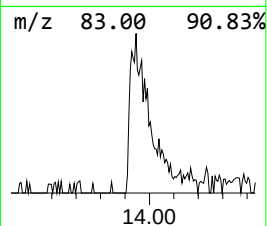
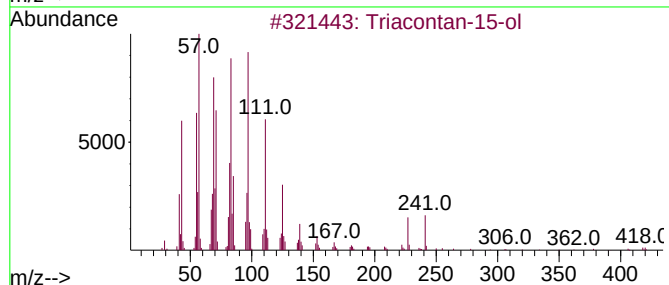
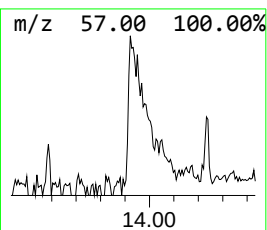
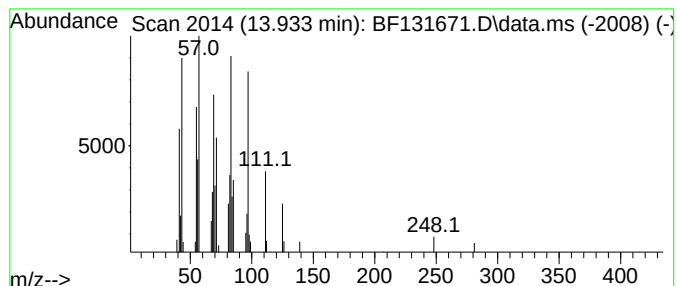
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Triacontan-15-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.933	2.06 ng	46032	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triacontan-15-ol	438	C30H62O	031849-26-0	90
2			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	90
3			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	90
4			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	90
5			1-Heneicosanol	312	C21H44O	015594-90-8	90



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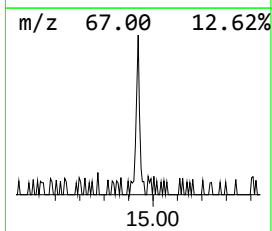
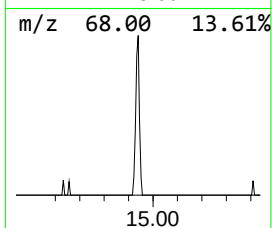
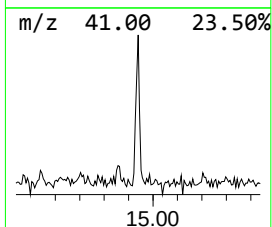
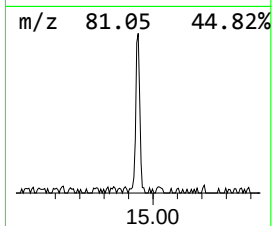
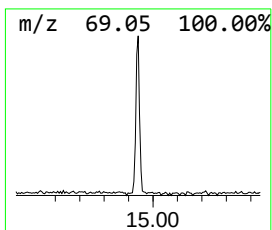
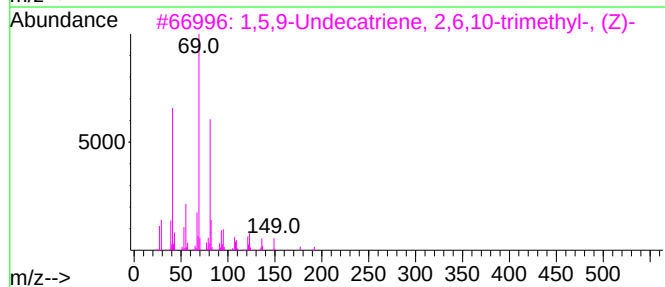
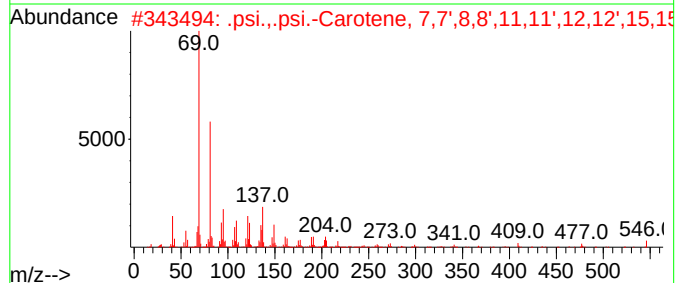
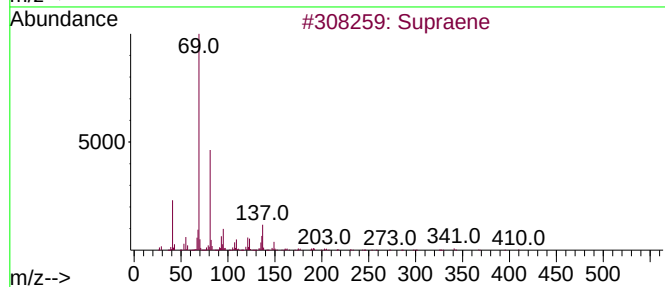
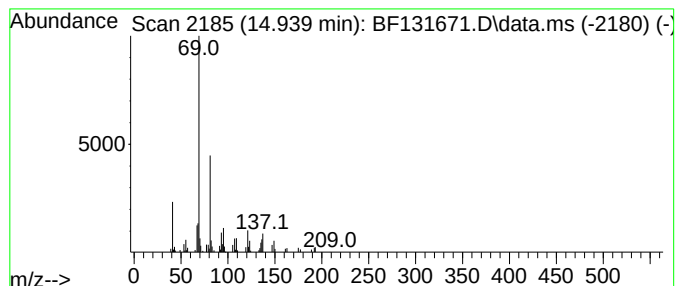
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.939	2.93 ng	57245	Perylene-d12	15.580

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	87
2			.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	83
3			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	80
4			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	78
5			2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	53



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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...	2.128	19.1	ng	382707	1	6.881	400903	20.0
2-Pentanone, 4-...	5.087	10.8	ng	215889	1	6.881	400903	20.0
Benzophenone	10.651	2.9	ng	81950	3	9.933	563740	20.0
Triacontan-15-ol	13.933	2.1	ng	46032	5	14.080	447382	20.0
Supraene	14.939	2.9	ng	57245	6	15.580	391241	20.0