

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060821\
 Data File : BF124189.D
 Acq On : 8 Jun 2021 20:10
 Operator : JU/CG
 Sample : M2598-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 23

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-BF060321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124189.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.140	3	9	17	rBB	494848	613623	50.60%	6.700%
2	2.969	144	150	156	rBB2	41695	64899	5.35%	0.709%
3	5.086	506	510	517	rVB3	11757	16764	1.38%	0.183%
4	5.498	576	580	590	rBV	985566	908122	74.89%	9.916%
5	6.510	748	752	770	rVB	865600	867260	71.52%	9.470%
6	6.863	808	812	815	rBV	324532	276179	22.78%	3.016%
7	7.422	902	907	910	rBV	649228	631530	52.08%	6.896%
8	8.145	1026	1030	1033	rBV	374052	331352	27.32%	3.618%
9	9.222	1208	1213	1216	rBV	1422786	1212634	100.00%	13.241%
10	9.557	1267	1270	1272	rBV	31225	23452	1.93%	0.256%
11	9.598	1272	1277	1286	rVB3	11454	15277	1.26%	0.167%
12	9.869	1318	1323	1325	rBV3	33272	35320	2.91%	0.386%
13	9.898	1325	1328	1331	rVB	484165	367935	30.34%	4.018%
14	10.686	1458	1462	1467	rBV	750242	662612	54.64%	7.235%
15	11.245	1554	1557	1560	rBV4	15872	15561	1.28%	0.170%
16	11.386	1577	1581	1584	rBV	385112	309088	25.49%	3.375%
17	11.410	1584	1585	1589	rVB	30534	18646	1.54%	0.204%
18	11.915	1669	1671	1673	rBV3	15221	17188	1.42%	0.188%
19	12.598	1785	1787	1790	rBV	20625	15319	1.26%	0.167%
20	12.827	1824	1826	1828	rBV2	20039	14669	1.21%	0.160%
21	12.974	1846	1851	1854	rBV	1080427	904566	74.60%	9.877%
22	13.204	1887	1890	1891	rBV2	14517	16236	1.34%	0.177%
23	13.451	1928	1932	1935	rVB	682636	620738	51.19%	6.778%
24	14.027	2024	2030	2034	rBV	287209	296750	24.47%	3.240%
25	14.233	2063	2065	2068	rVB3	18436	13807	1.14%	0.151%
26	14.804	2160	2162	2165	rBV4	16908	17369	1.43%	0.190%
27	15.086	2206	2210	2211	rBV4	25099	23586	1.95%	0.258%
28	15.151	2217	2221	2224	rVB	93314	102212	8.43%	1.116%
29	15.515	2278	2283	2291	rVB2	215104	303292	25.01%	3.312%
30	15.721	2316	2318	2319	rBV2	16904	13658	1.13%	0.149%
31	15.974	2357	2361	2368	rVB2	225781	342010	28.20%	3.735%
32	16.174	2393	2395	2398	rVB4	20773	22340	1.84%	0.244%
33	17.086	2547	2550	2558	rVB9	28833	64022	5.28%	0.699%

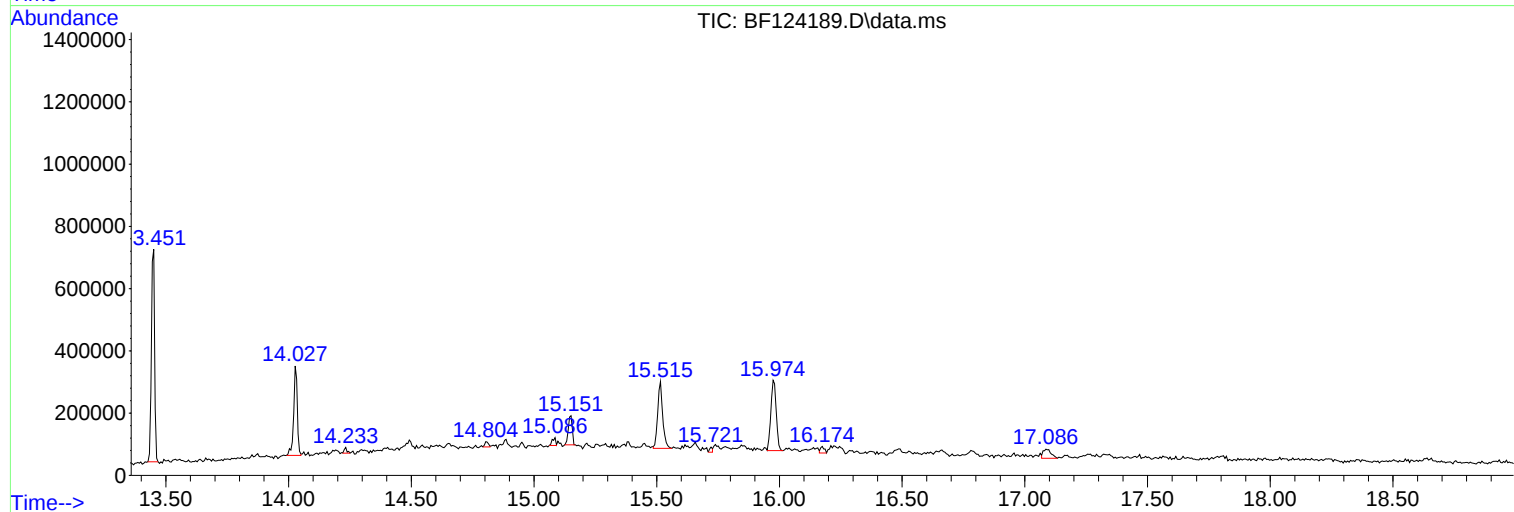
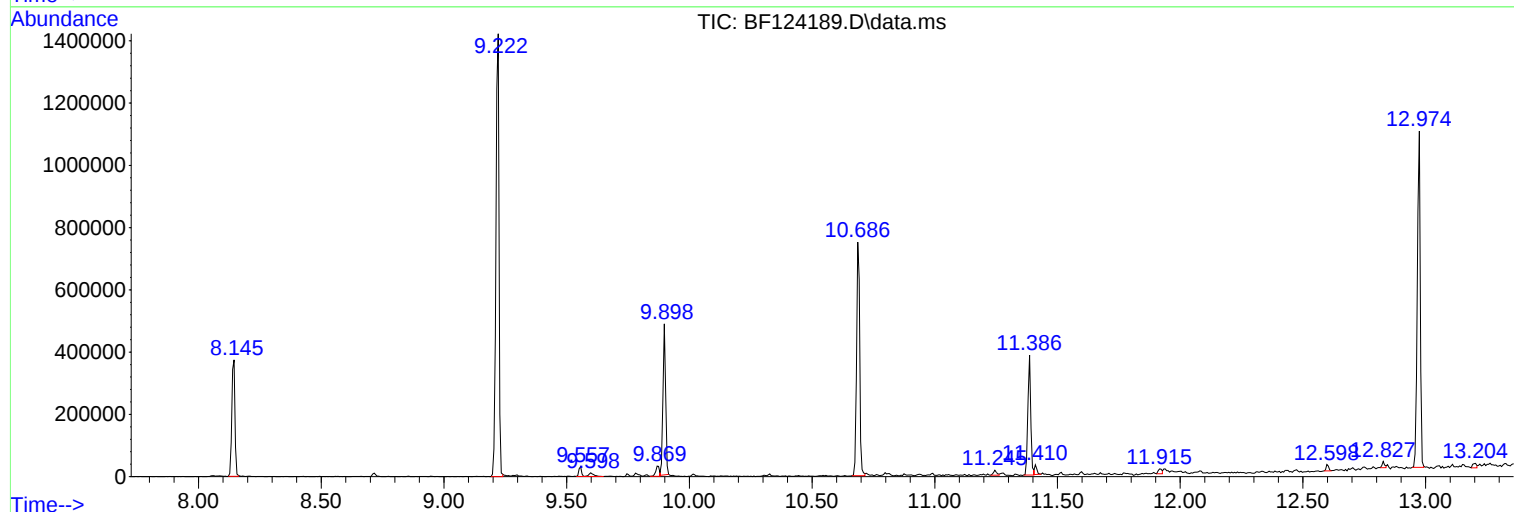
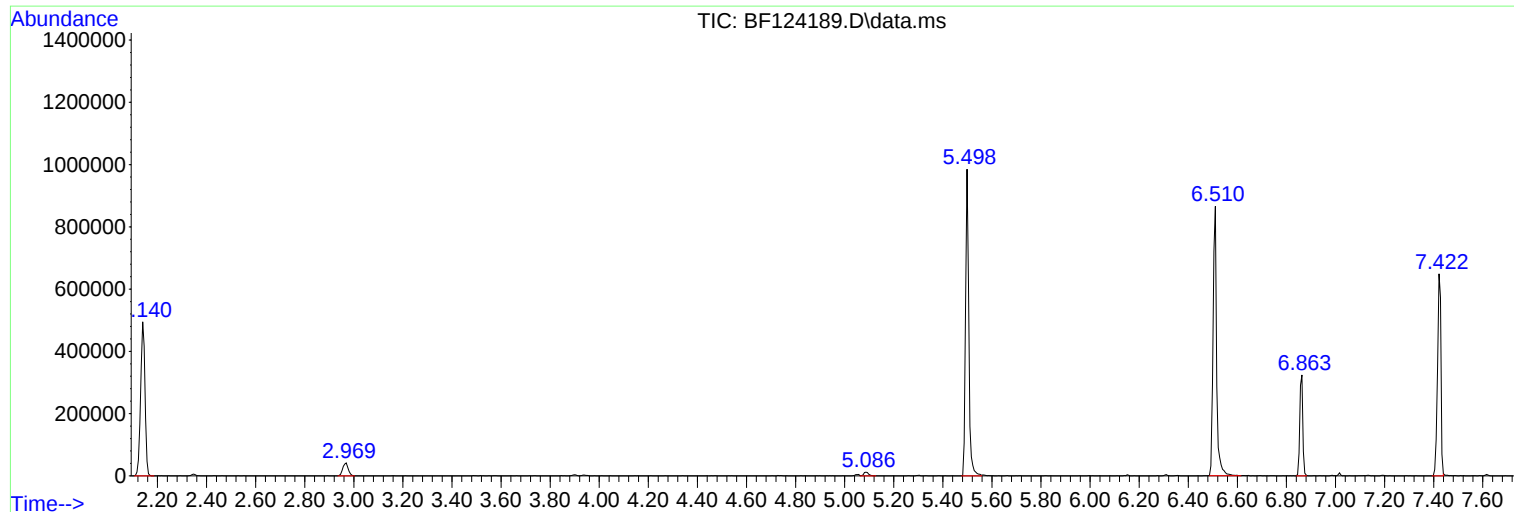
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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ClientSampled :
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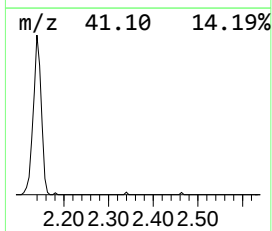
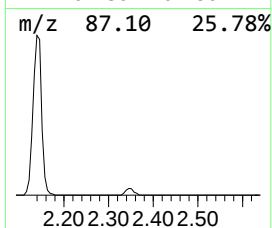
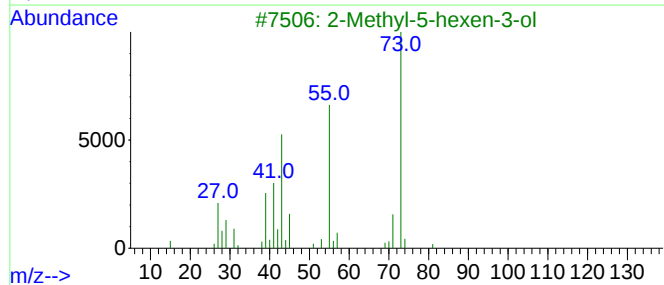
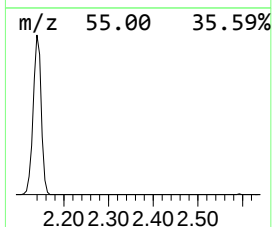
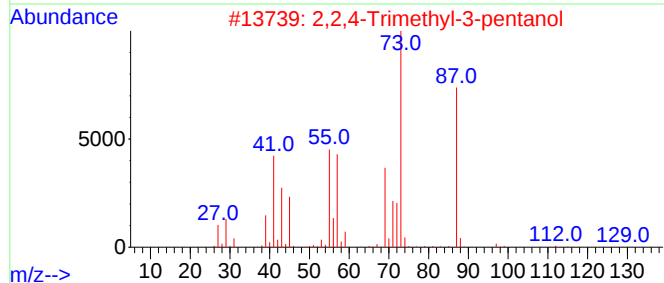
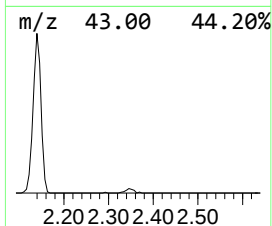
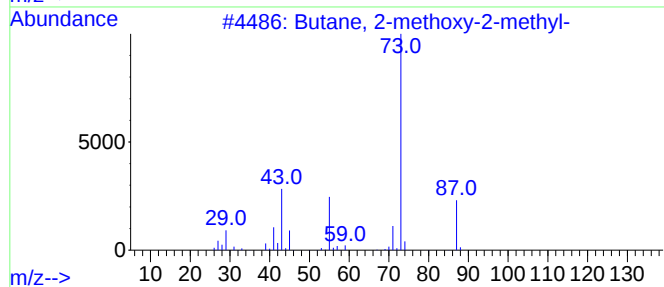
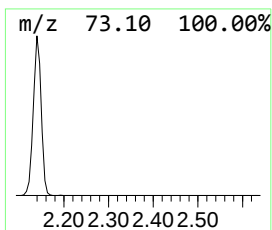
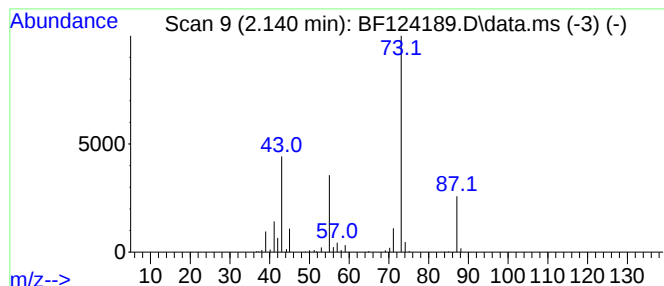
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.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.
2.140	44.44 ng	613623	1,4-Dichlorobenzene-d4	6.863

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			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	37
4			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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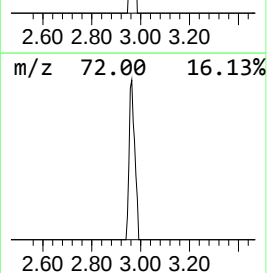
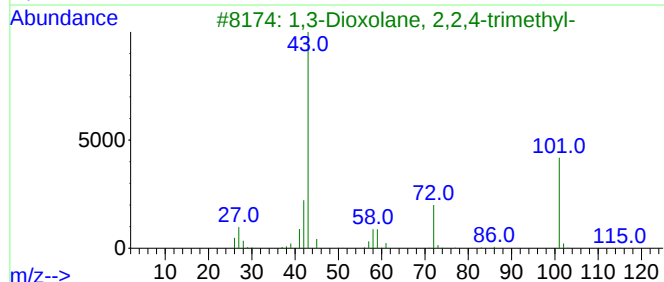
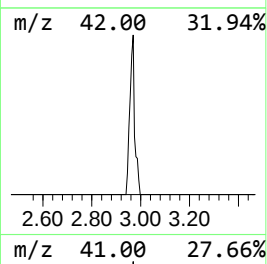
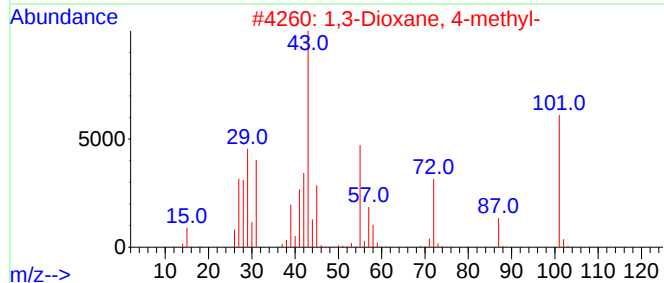
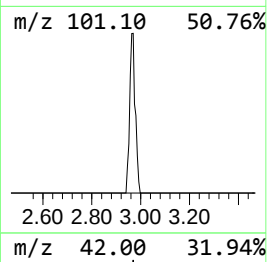
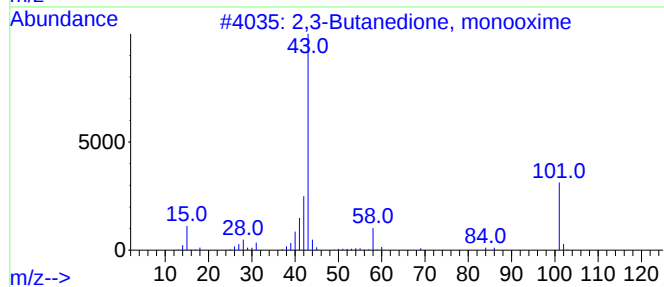
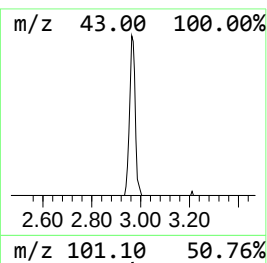
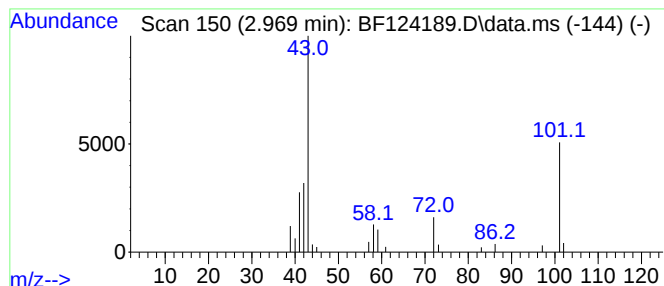
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2,3-Butanedione, monooxime Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.969	4.70 ng	64899	1,4-Dichlorobenzene-d4	6.863

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	59
2		1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	59
3		1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	56
4		Butane	58	C4H10	000106-97-8	10
5		Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	9



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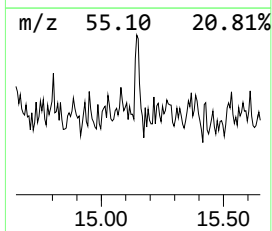
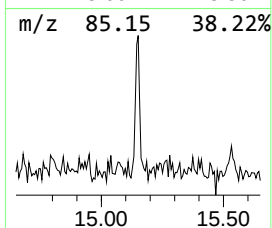
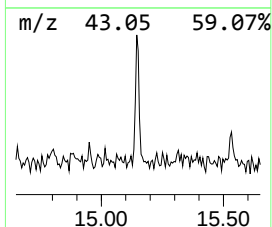
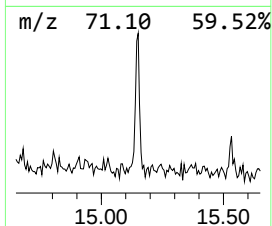
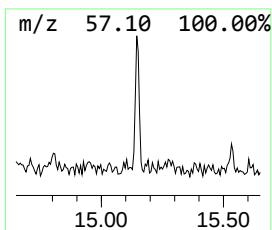
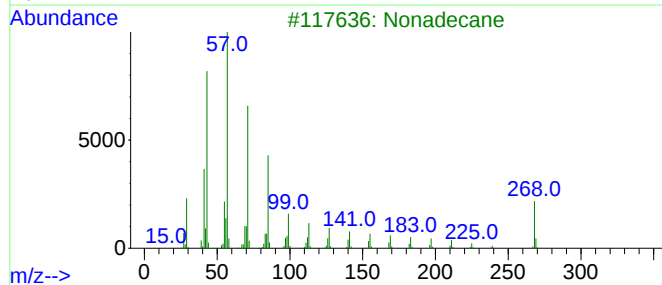
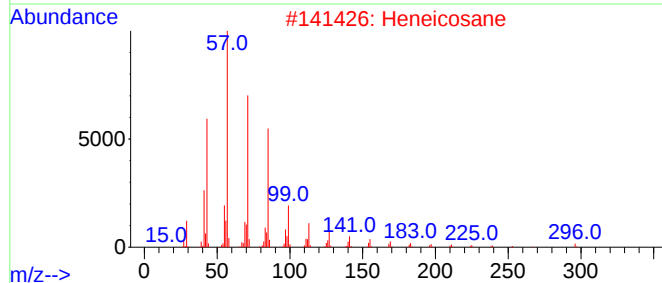
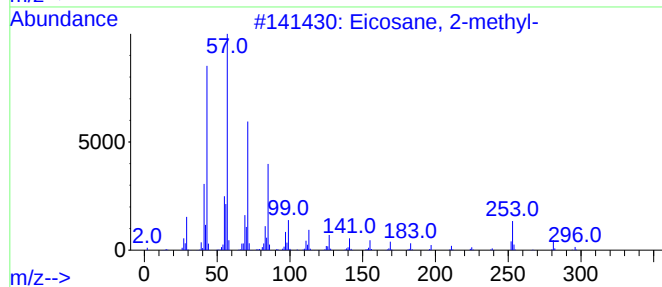
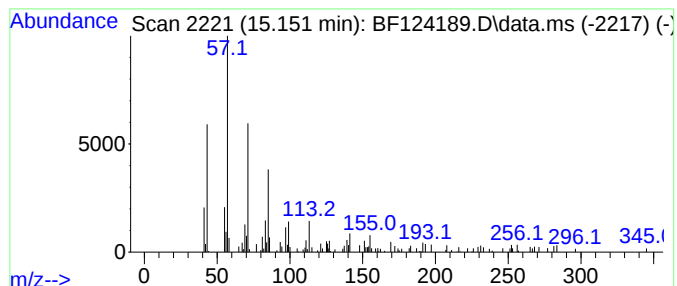
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Eicosane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.150	6.74 ng	102212	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane, 2-methyl-	296	C21H44	001560-84-5	93
2			Heneicosane	296	C21H44	000629-94-7	91
3			Nonadecane	268	C19H40	000629-92-5	91
4			Behenyl chloride	344	C22H45Cl	042217-03-8	90
5			Tetratetracontane	619	C44H90	007098-22-8	87



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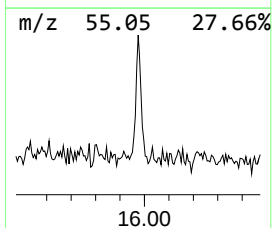
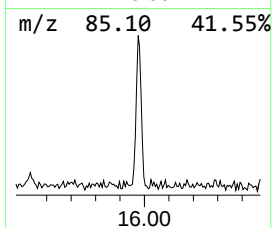
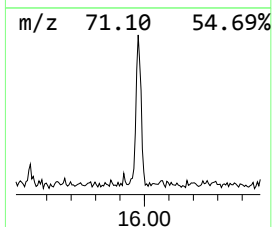
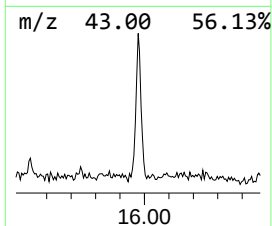
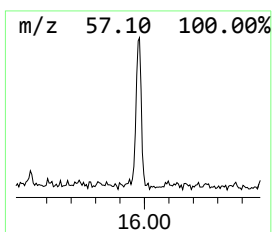
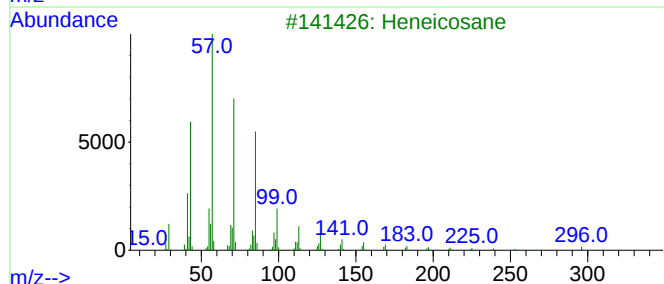
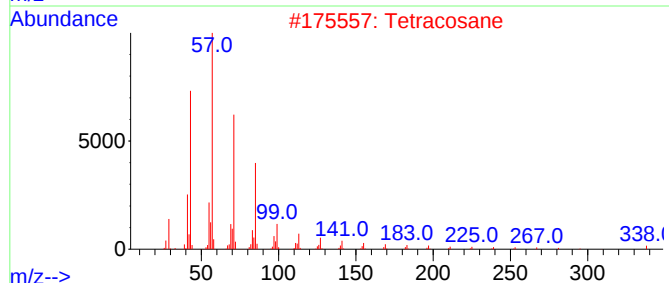
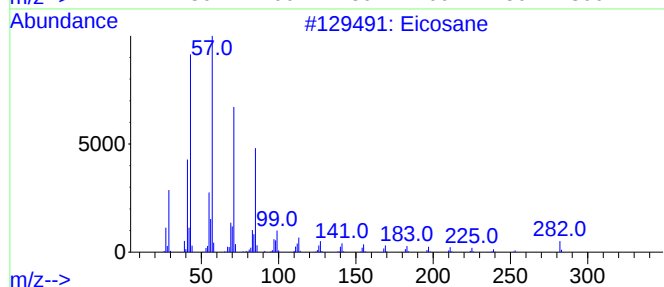
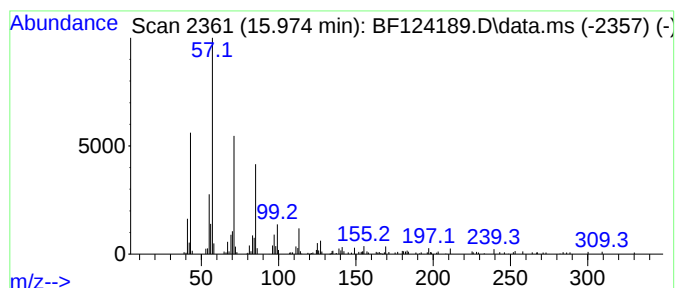
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Eicosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.974	22.55 ng	342010	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane			282	C20H42	000112-95-8	95
2	Tetracosane			338	C24H50	000646-31-1	90
3	Heneicosane			296	C21H44	000629-94-7	87
4	Pentacosane			352	C25H52	000629-99-2	87
5	Octacosane			394	C28H58	000630-02-4	87



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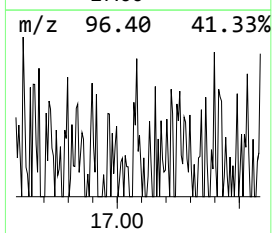
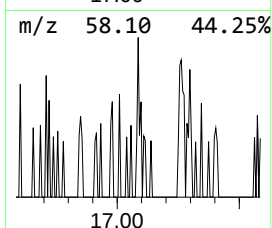
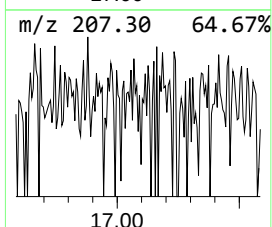
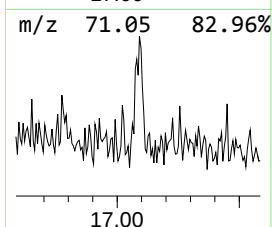
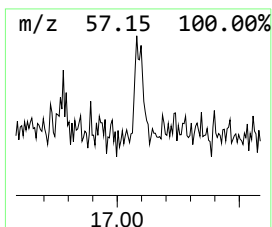
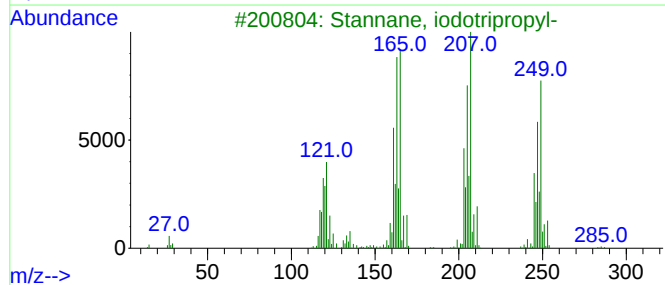
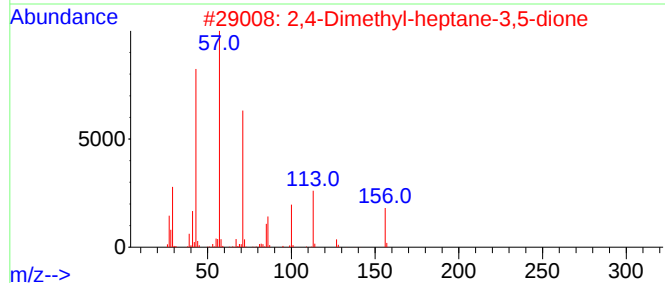
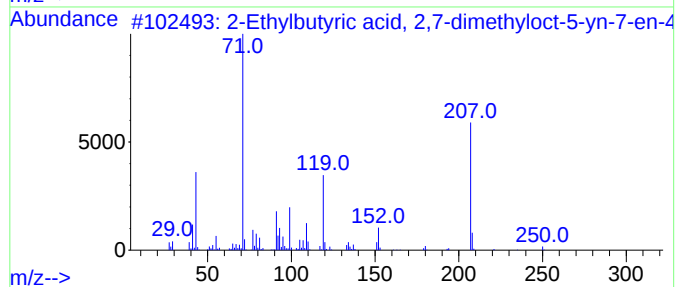
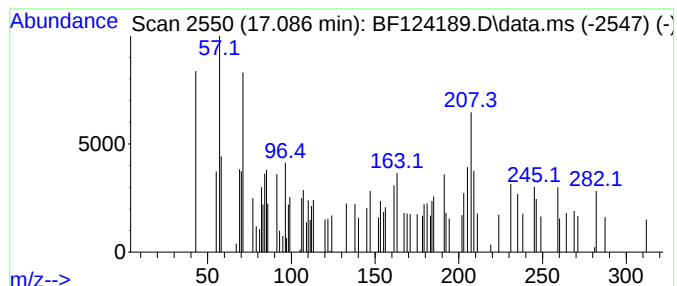
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TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown17.086 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.086	4.22 ng	64022	Perylene-d12	15.515	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Ethylbutyric acid, 2,7-dimethy...	250	C16H26O2	1000371-19-7	22
2	2,4-Dimethyl-heptane-3,5-dione	156	C9H16O2	037484-68-7	18
3	Stannane, iodotripropyl-	376	C9H21ISn	007342-45-2	14
4	6-Hydroxy-9-oxa-bicyclo[3.3.1]no...	156	C8H12O3	1000194-46-8	14
5	Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	10



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.140	44.4	ng	613623	1	6.863	276179	20.0
2,3-Butanedione...	2.969	4.7	ng	64899	1	6.863	276179	20.0
Eicosane, 2-met...	15.150	6.7	ng	102212	6	15.515	303292	20.0
Eicosane	15.974	22.6	ng	342010	6	15.515	303292	20.0
unknown17.086	17.086	4.2	ng	64022	6	15.515	303292	20.0