LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121124\
Data File : BF140828.D
Acq On : 11 Dec 2024 14:42
Operator : RC/JU
Sample : PB165479BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB165479BL

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-BF112124.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140828.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.234	18	24	35	rVB	568071	1332910	41.13%	7.494%
2	5.104	505	512	529	rBV	609267	940996	29.04%	5.290%
3	5.510	576	581	604	rBV	1020535	1413765	43.63%	7.948%
4	5.681	605	610	621	rVB3	48627	79169	2.44%	0.445%
5	6.128	681	686	701	rBV	81006	117245	3.62%	0.659%
6	6.510	745	751	778	rBV	1061932	1488116	45.92%	8.366%
7	6.857	805	810	816	rBV	364767	454860	14.04%	2.557%
8	7.016	834	837	854	rVB2	75744	121629	3.75%	0.684%
9	7.428	900	907	925	rBV	1010610	1455330	44.91%	8.182%
10	8.139	1022	1028	1043	rBV	442881	590971	18.24%	3.322%
11	9.216	1204	1211	1235	rBV	2120853	2904635	89.64%	16.330%
12	9.898	1321	1327	1344	rBV	507224	683048	21.08%	3.840%
13	10.692	1457	1462	1490	rBV	762655	1055857	32.58%	5.936%
14	11.392	1575	1581	1605	rBV	566962	781321	24.11%	4.393%
15	12.980	1845	1851	1856	rBV	2426657	3240391	100.00%	18.218%
16	14.045	2027	2032	2044	rBV	388886	592253	18.28%	3.330%
17	15.557	2283	2289	2305	rVB	231583	443531	13.69%	2.494%
18	15.986	2358	2362	2373	rVB2	23773	45229	1.40%	0.254%
19	16.498	2445	2449	2457	rVB	23192	45762	1.41%	0.257%

Sum of corrected areas: 17787018

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ClientSampleId :
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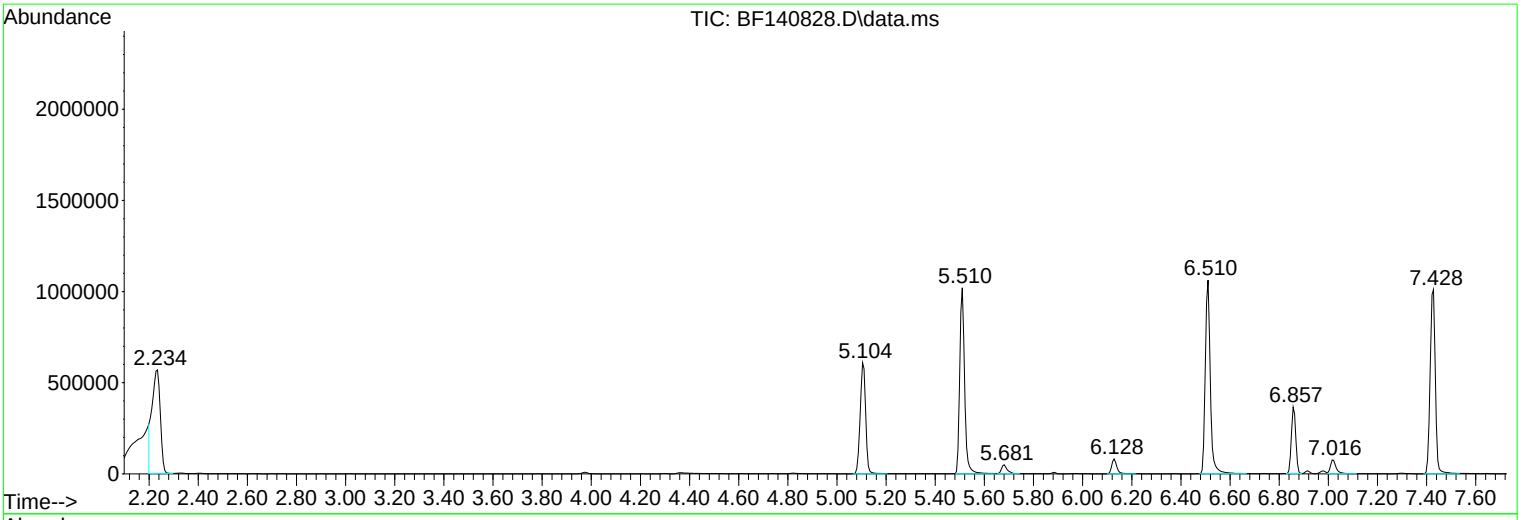
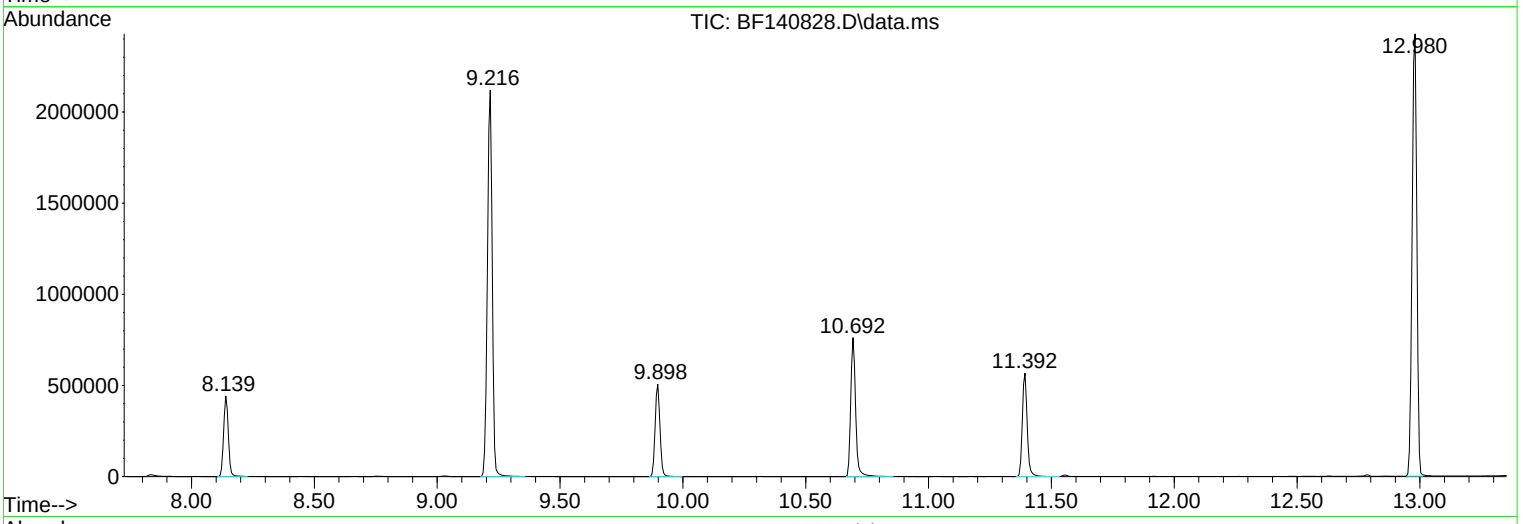
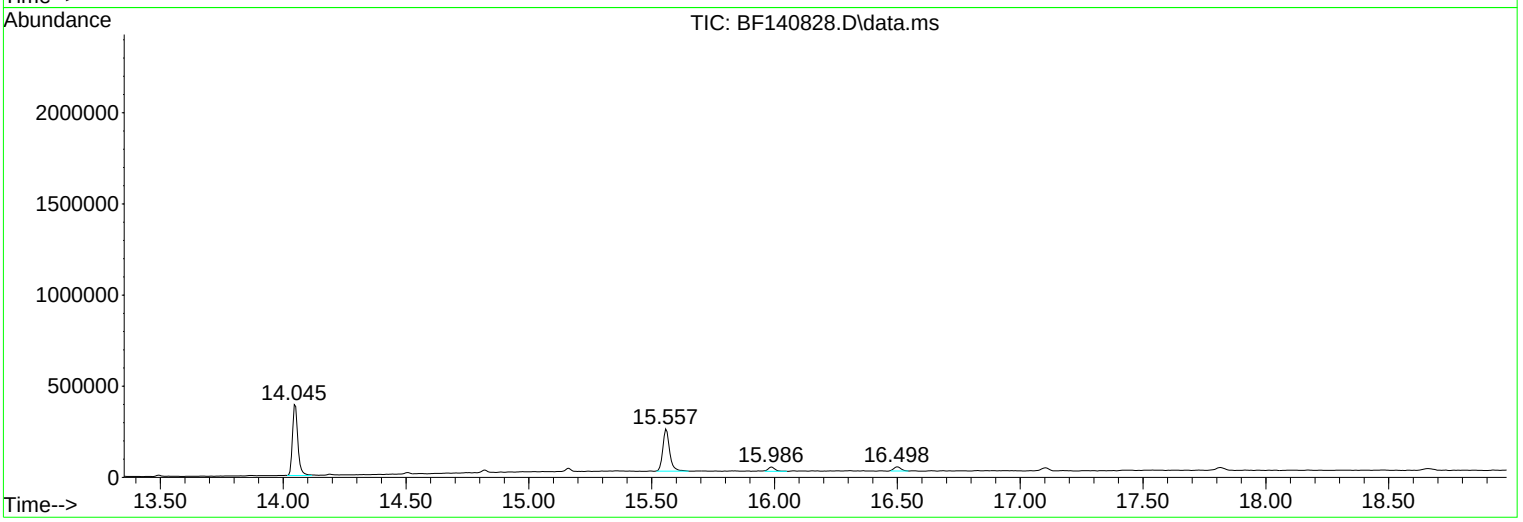
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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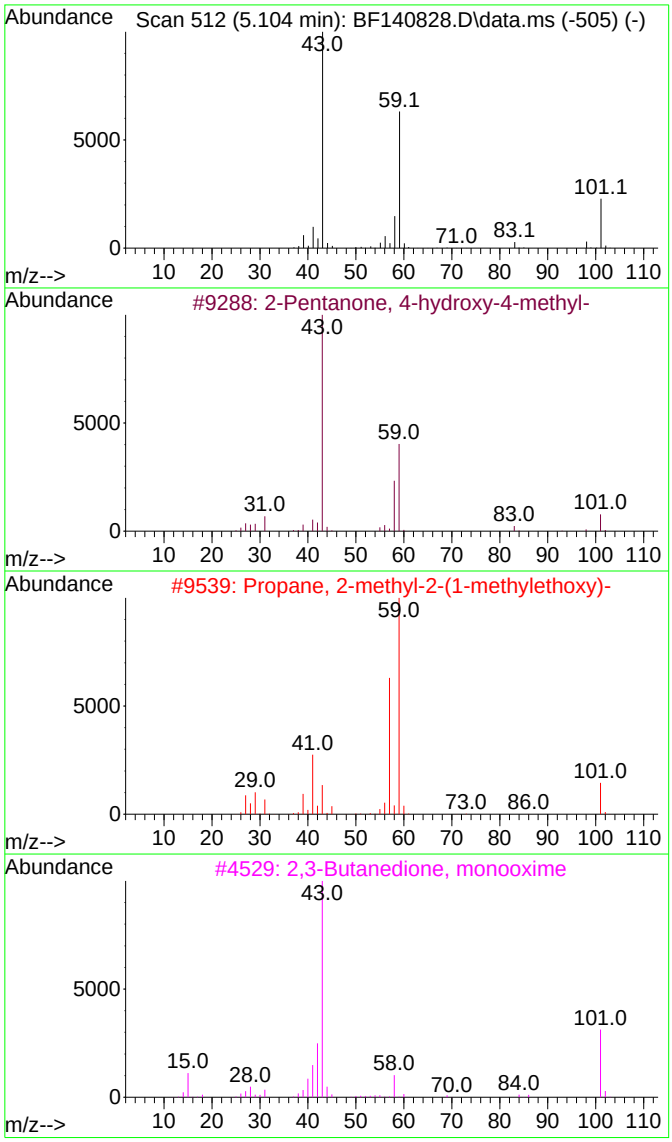
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

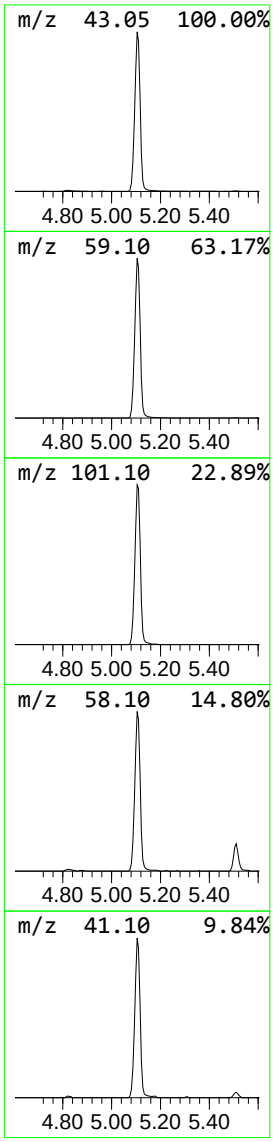
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	41.38 ng	940996	1,4-Dichlorobenzene-d4	6.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
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	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.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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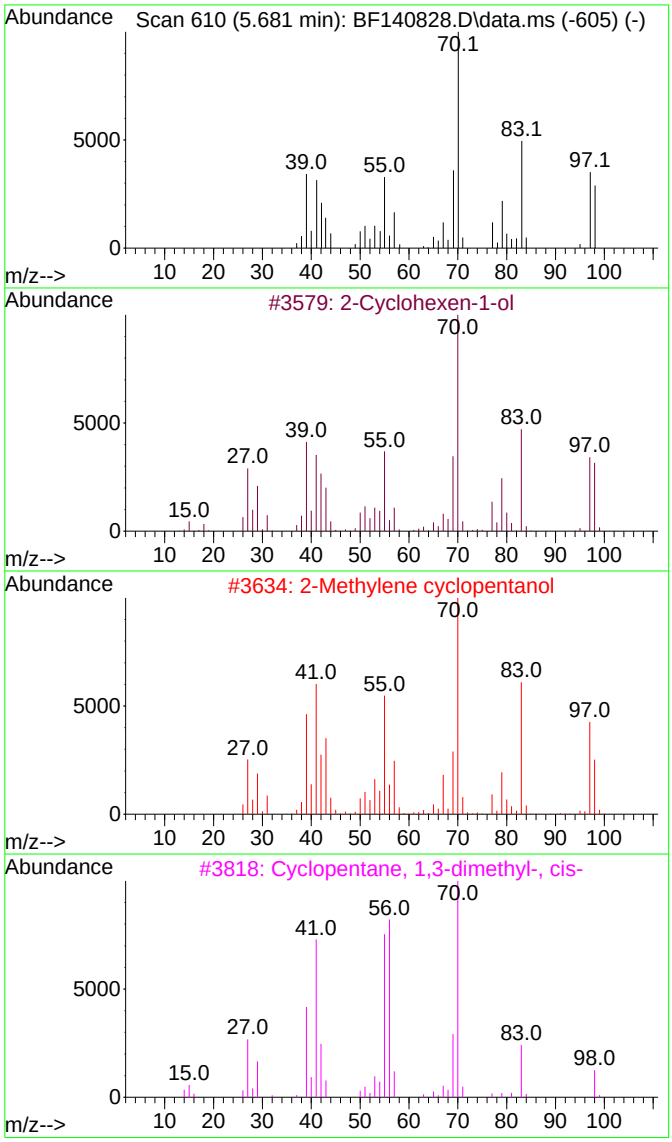
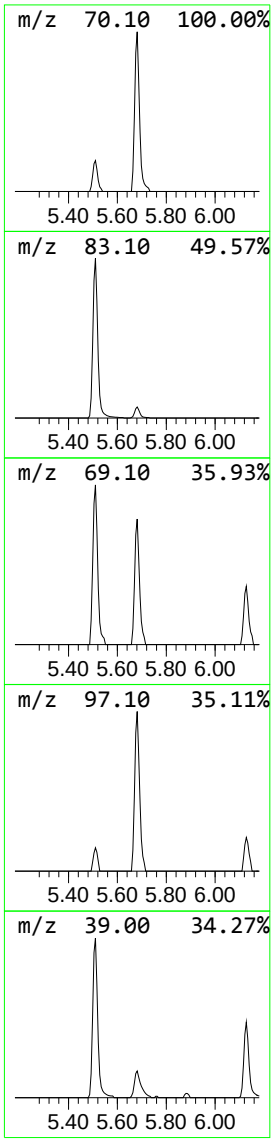
Peak Number 3 2-Cyclohexen-1-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.681	3.48 ng	79169	1,4-Dichlorobenzene-d4	6.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclohexen-1-ol	98	C6H10O	000822-67-3	96
2	2-Methylene cyclopentanol	98	C6H10O	020461-31-8	50
3	Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	38
4	Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	37
5	2,6-Cyclooctadien-1-ol	124	C8H12O	010017-18-2	32





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Operator : RC/JU
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Misc :
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Instrument :
BNA_F
ClientSampleId :
PB165479BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.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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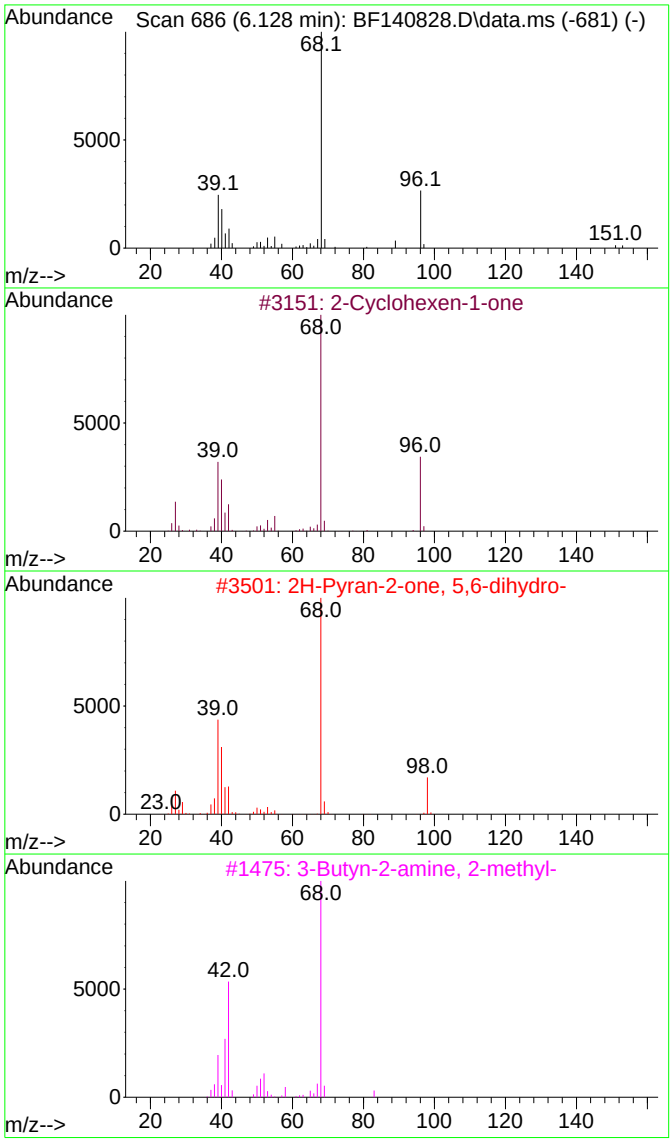
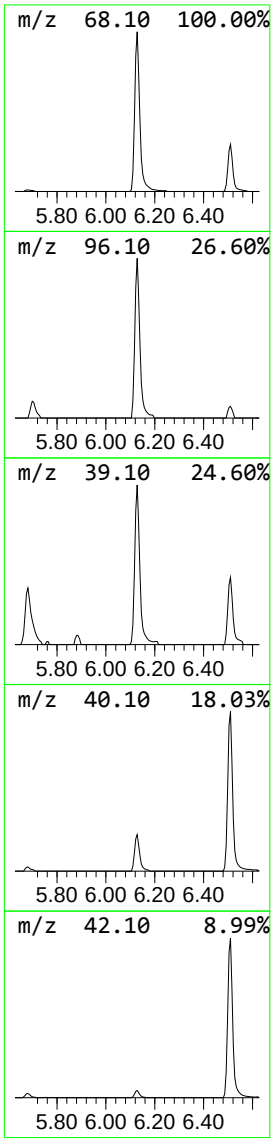
Peak Number 4 2-Cyclohexen-1-one Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.128	5.16 ng	117245	1,4-Dichlorobenzene-d4	6.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	90
2	2H-Pyran-2-one, 5,6-dihydro-	98	C5H6O2	003393-45-1	50
3	3-Butyn-2-amine, 2-methyl-	83	C5H9N	002978-58-7	42
4	5,6-Dihydro-2(1H)-pyridinone	97	C5H7NO	006052-73-9	40
5	1,5-Cyclooctadien-4-one	122	C8H10O	001460-21-5	40





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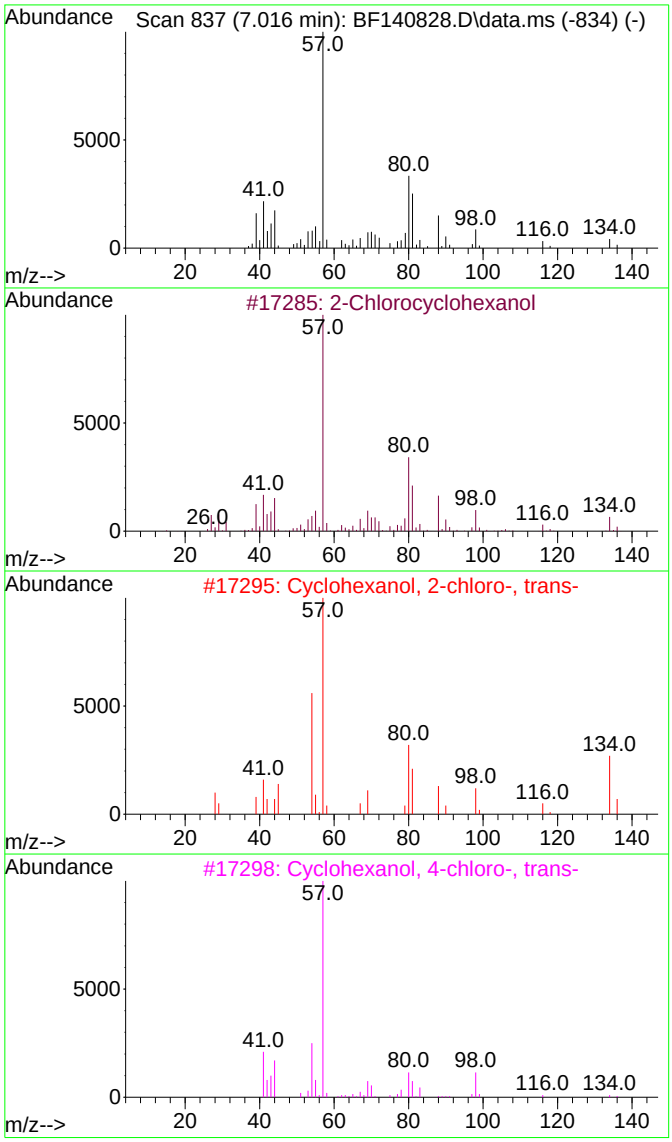
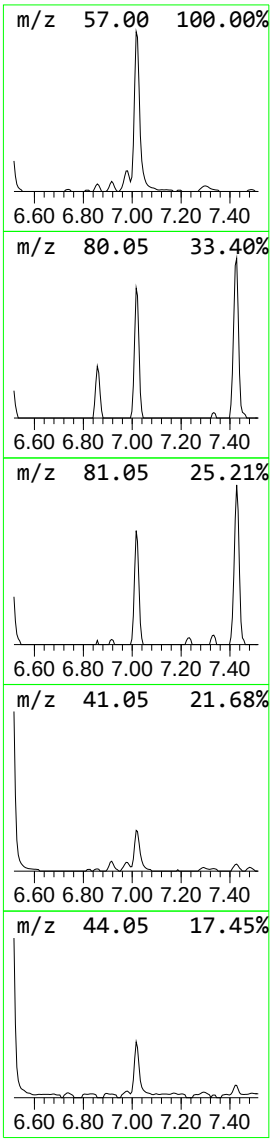
Peak Number 5 2-Chlorocyclohexanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.016	5.35 ng	121629	1,4-Dichlorobenzene-d4	6.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Chlorocyclohexanol	134	C6H11ClO	001561-86-0	94
2	Cyclohexanol, 2-chloro-, trans-	134	C6H11ClO	006628-80-4	37
3	Cyclohexanol, 4-chloro-, trans-	134	C6H11ClO	029538-77-0	35
4	3-Furanol, tetrahydro-	88	C4H8O2	000453-20-3	25
5	Oxalic acid, isobutyl heptyl ester	244	C13H24O4	1000309-37-2	14





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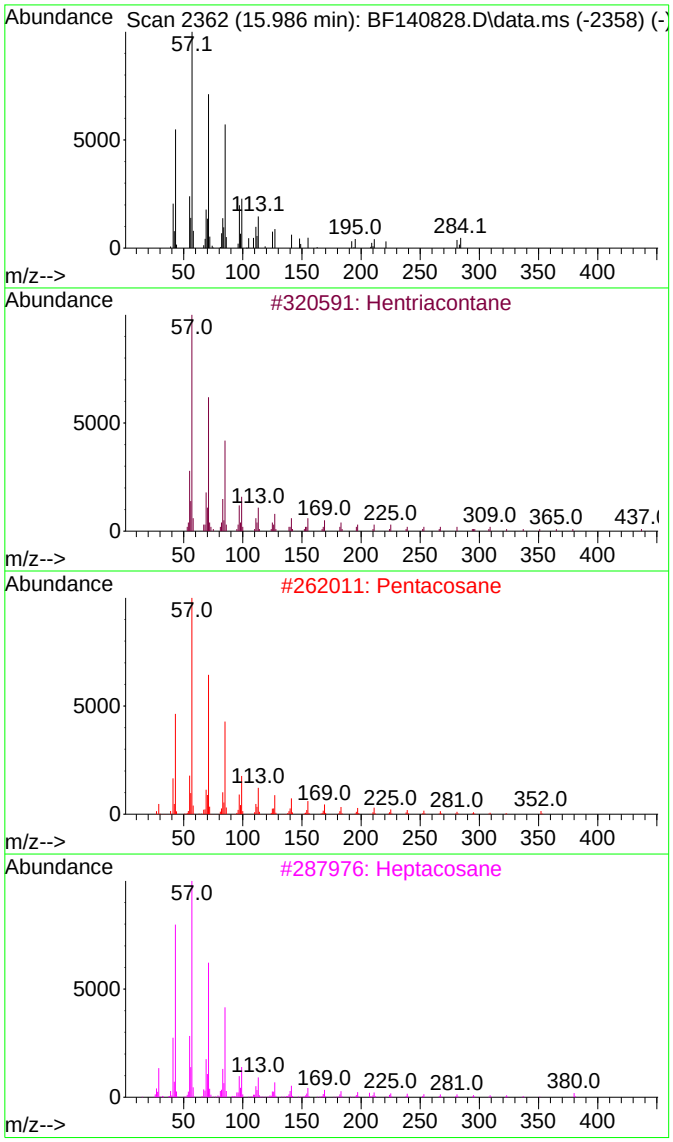
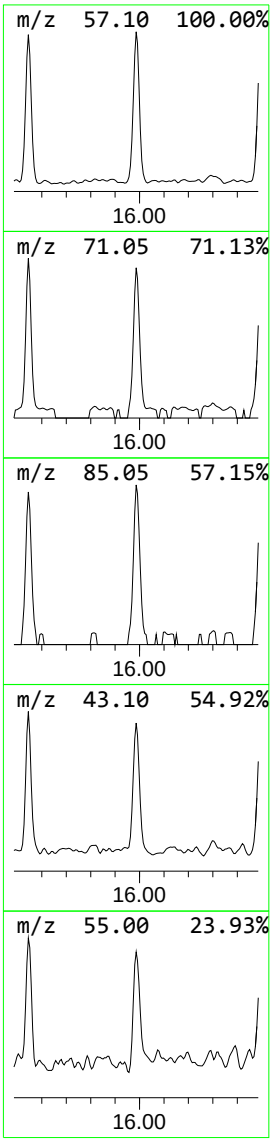
Peak Number 6 Hentriacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.986	2.04 ng	45229	Perylene-d12	15.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	87
2	Pentacosane	352	C25H52	000629-99-2	86
3	Heptacosane	380	C27H56	000593-49-7	83
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	80
5	Heneicosane	296	C21H44	000629-94-7	74





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TIC Library : C:\Database\NIST20.L
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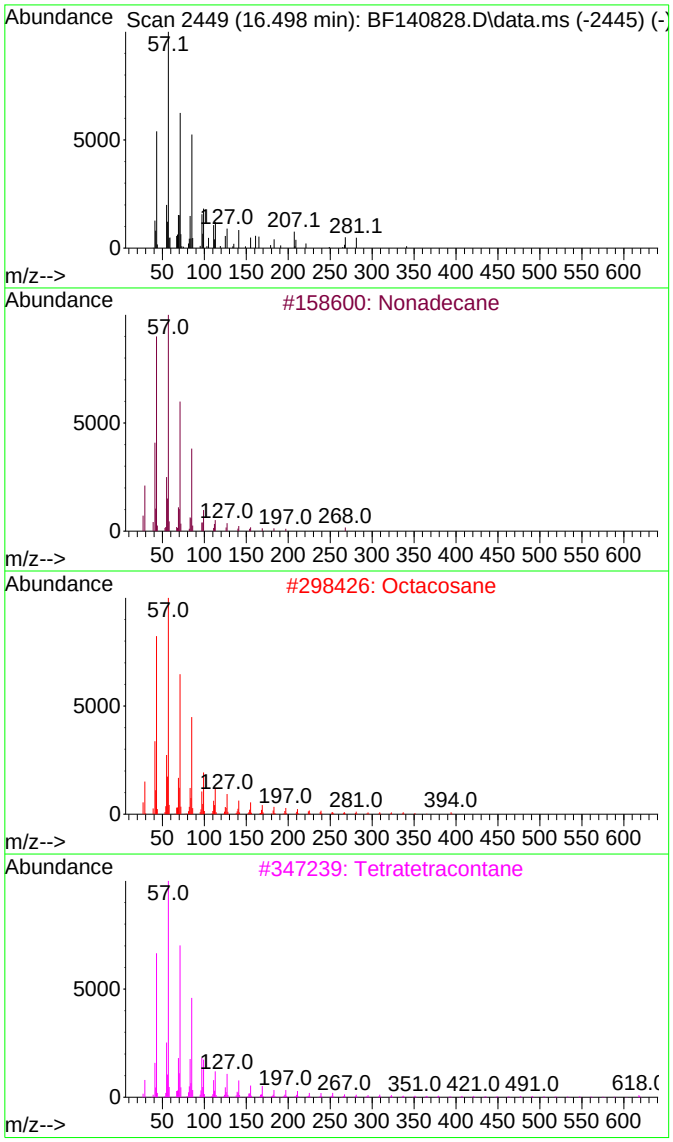
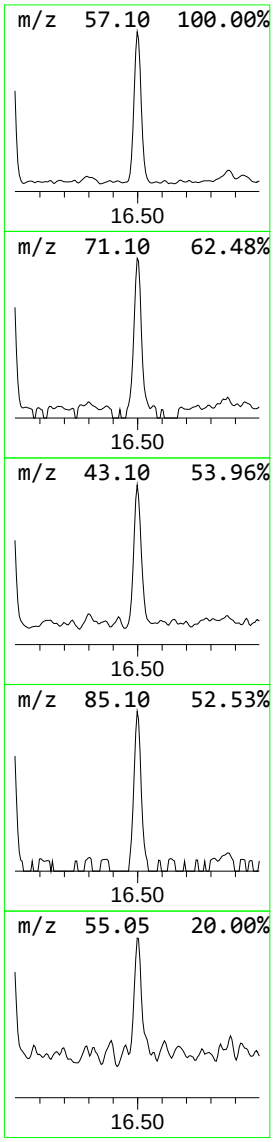
Peak Number 7 Nonadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.498	2.06 ng	45762	Perylene-d12	15.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Tetratetracontane	619	C44H90	007098-22-8	90
4	Tetracosane	338	C24H50	000646-31-1	90
5	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	87





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	5.104	41.4	ng	940996	1	6.857	454860	20.0
2-Cyclohexen-1-ol	5.681	3.5	ng	79169	1	6.857	454860	20.0
2-Cyclohexen-1-one	6.128	5.2	ng	117245	1	6.857	454860	20.0
2-Chlorocyclohe...	7.016	5.3	ng	121629	1	6.857	454860	20.0
Hentriacontane	15.986	2.0	ng	45229	6	15.557	443531	20.0
Nonadecane	16.498	2.1	ng	45762	6	15.557	443531	20.0