LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111424\
Data File : BF140355.D
Acq On : 14 Nov 2024 11:27
Operator : RC/JU
Sample : PB164911BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB164911BL

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-BF111324.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140355.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	3	29	36	rBV	1071295	4219798	79.90%	12.222%
2	4.251	361	367	376	rBV2	23017	66170	1.25%	0.192%
3	5.110	505	513	534	rBV	1266237	1967475	37.25%	5.698%
4	5.504	574	580	585	rBV	2044460	2684697	50.83%	7.776%
5	5.687	605	611	620	rBV2	97621	156579	2.96%	0.453%
6	6.128	681	686	698	rVB	189146	251122	4.75%	0.727%
7	6.498	743	749	754	rBV	2079065	2861079	54.17%	8.286%
8	6.875	808	813	818	rBV	708758	866954	16.41%	2.511%
9	7.028	834	839	853	rVB	168464	233135	4.41%	0.675%
10	7.434	902	908	914	rBV	1869648	2742979	51.93%	7.944%
11	7.781	960	967	984	rBV	34873	66606	1.26%	0.193%
12	8.157	1025	1031	1048	rVB	859344	1157331	21.91%	3.352%
13	9.228	1206	1213	1219	rBV	3661378	5118193	96.91%	14.824%
14	9.910	1323	1329	1344	rVB	1036795	1333820	25.25%	3.863%
15	10.698	1457	1463	1488	rBV	1396866	1859075	35.20%	5.384%
16	11.398	1577	1582	1604	rVB	1166903	1473590	27.90%	4.268%
17	12.986	1846	1852	1858	rBV	3860767	5281609	100.00%	15.297%
18	14.051	2026	2033	2051	rBV	754011	994665	18.83%	2.881%
19	15.198	2223	2228	2235	rVB	35696	54508	1.03%	0.158%
20	15.557	2283	2289	2304	rVB	458300	816675	15.46%	2.365%
21	16.033	2364	2370	2378	rBV	44295	79637	1.51%	0.231%
22	16.551	2451	2458	2466	rBV	43840	90473	1.71%	0.262%
23	17.156	2553	2561	2576	rBV	32074	81033	1.53%	0.235%
24	17.874	2676	2683	2700	rVB3	24801	70357	1.33%	0.204%

Sum of corrected areas: 34527560

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Instrument :
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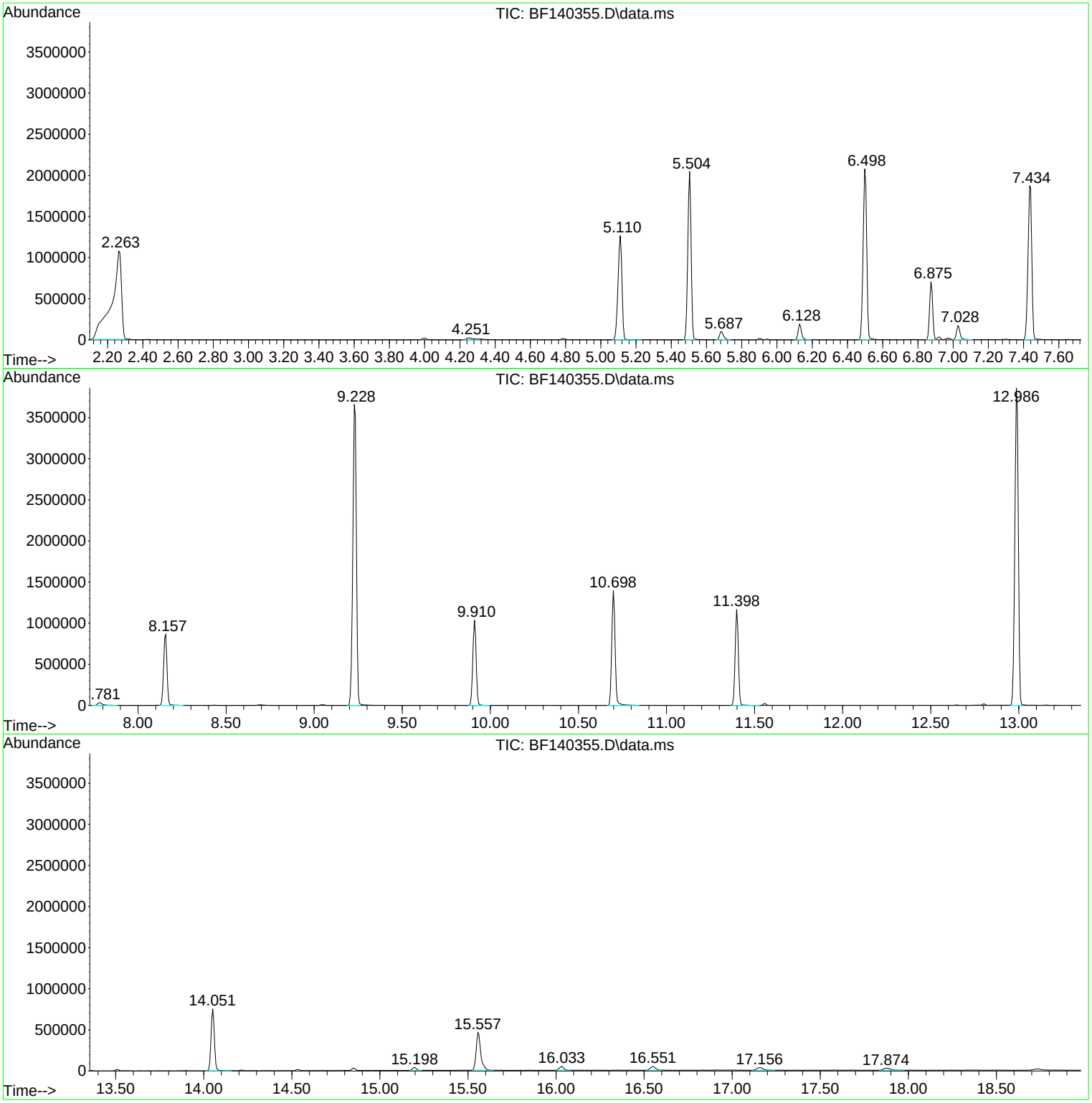
ClientSampleId :
PB164911BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.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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ClientSampleId :
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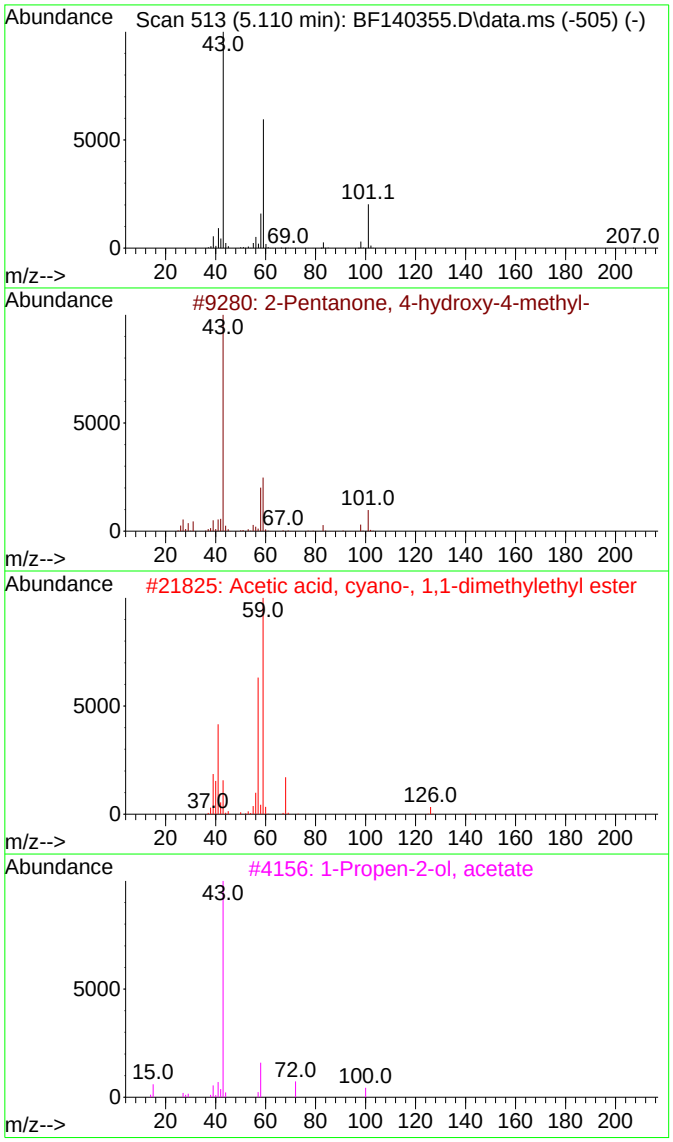
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

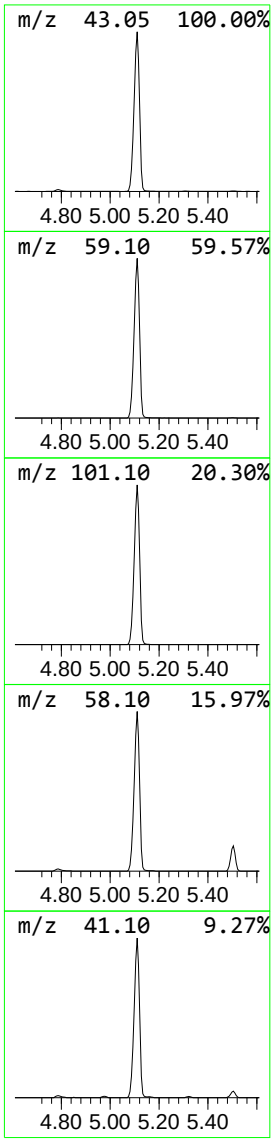
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	45.39 ng	1967480	1,4-Dichlorobenzene-d4	6.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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BNA_F
ClientSampleId :
PB164911BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

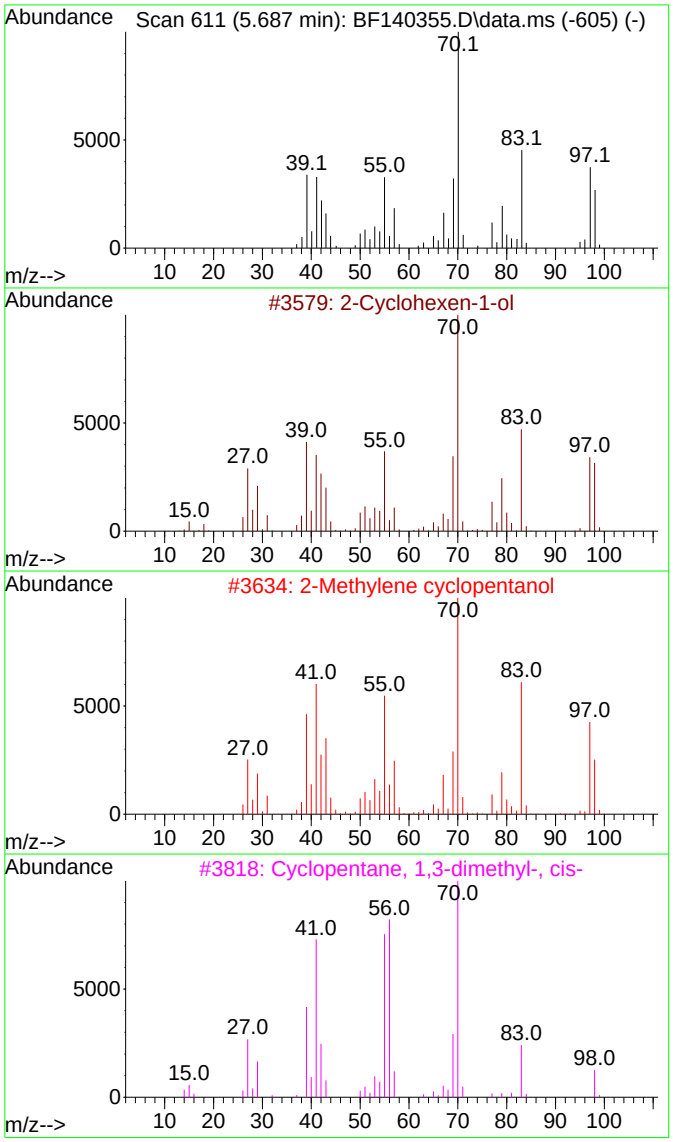
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

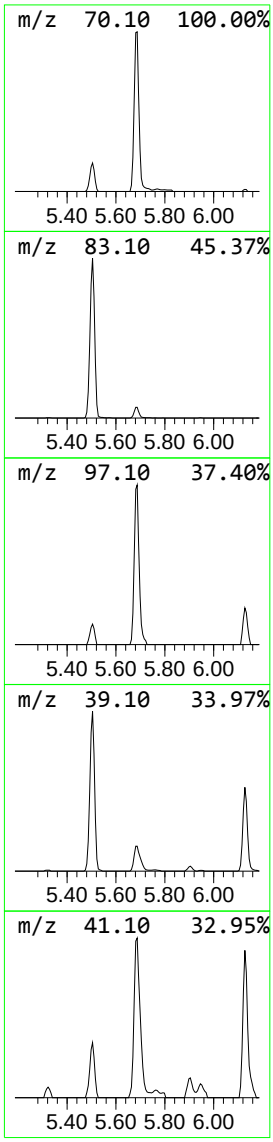
****

Peak Number 3 2-Cyclohexen-1-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.687	3.61 ng	156579	1,4-Dichlorobenzene-d4	6.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclohexen-1-ol	98	C6H10O	000822-67-3	94
2	2-Methylene cyclopentanol	98	C6H10O	020461-31-8	56
3	Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	37
4	Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	32
5	Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	32





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Sample : PB164911BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB164911BL

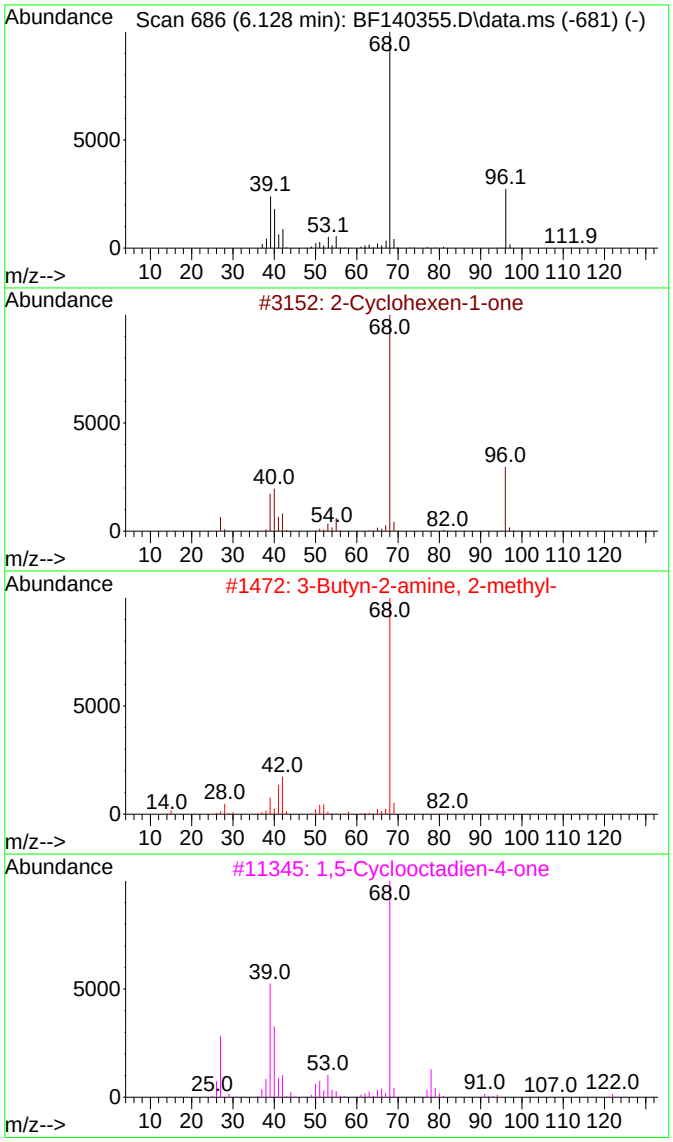
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

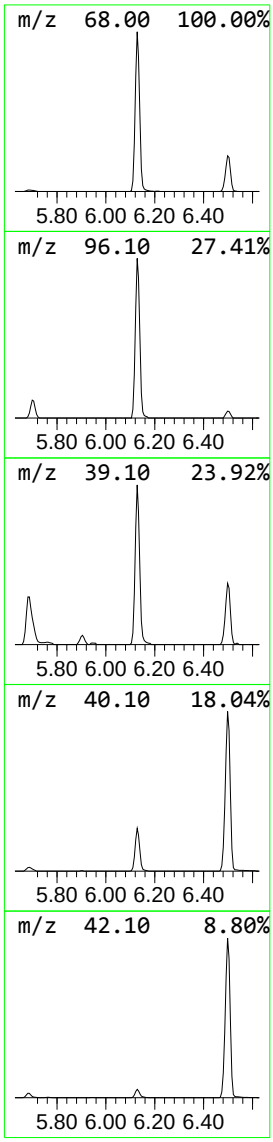
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Cyclohexen-1-one Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.128	5.79 ng	251122	1,4-Dichlorobenzene-d4	6.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	91
2	3-Butyn-2-amine, 2-methyl-	83	C5H9N	002978-58-7	36
3	1,5-Cyclooctadien-4-one	122	C8H10O	001460-21-5	33
4	Bicyclo[3.1.0]hexan-2-one	96	C6H8O	004160-49-0	12
5	2,5-Dihydro-3-methyl-thiophene 1...	132	C5H8O2S	001193-10-8	10





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BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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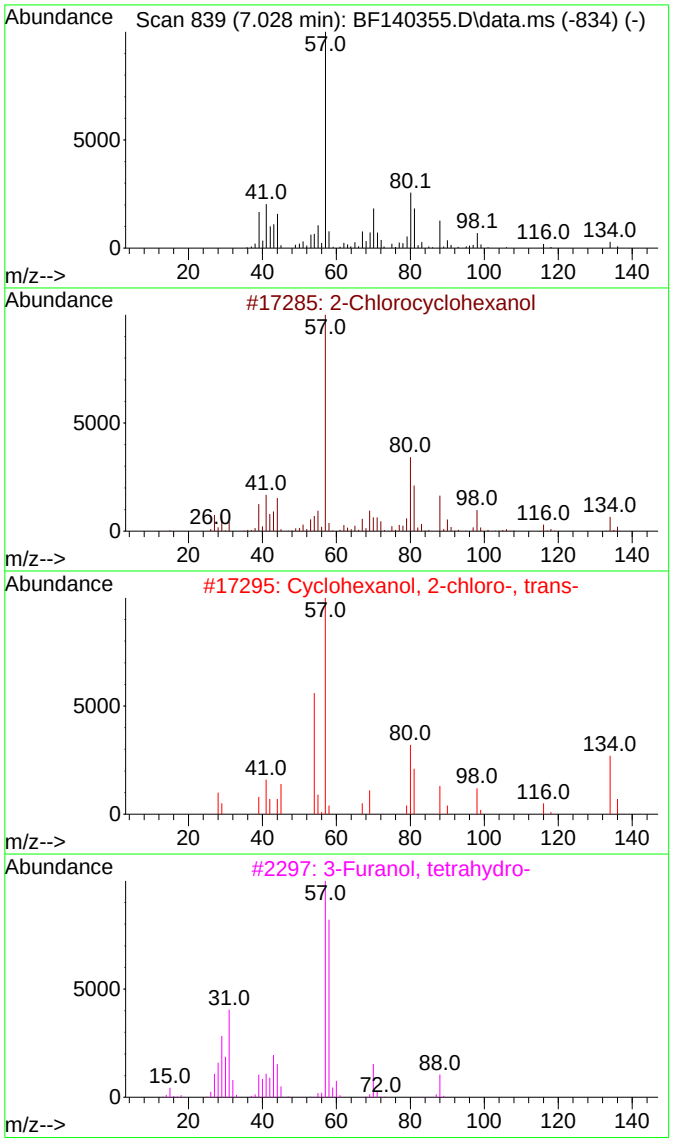
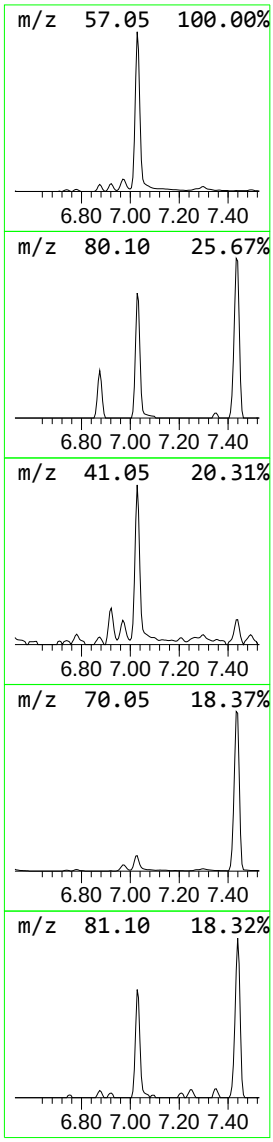
Peak Number 5 2-Chlorocyclohexanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.028	5.38 ng	233135	1,4-Dichlorobenzene-d4	6.875

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	38
3	3-Furanol, tetrahydro-	88	C4H8O2	000453-20-3	38
4	Butanoic acid, 2-hydroxy-3,3-dim...	132	C6H12O3	004026-20-4	16
5	Oxalic acid, isobutyl heptyl ester	244	C13H24O4	1000309-37-2	14





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111324.M
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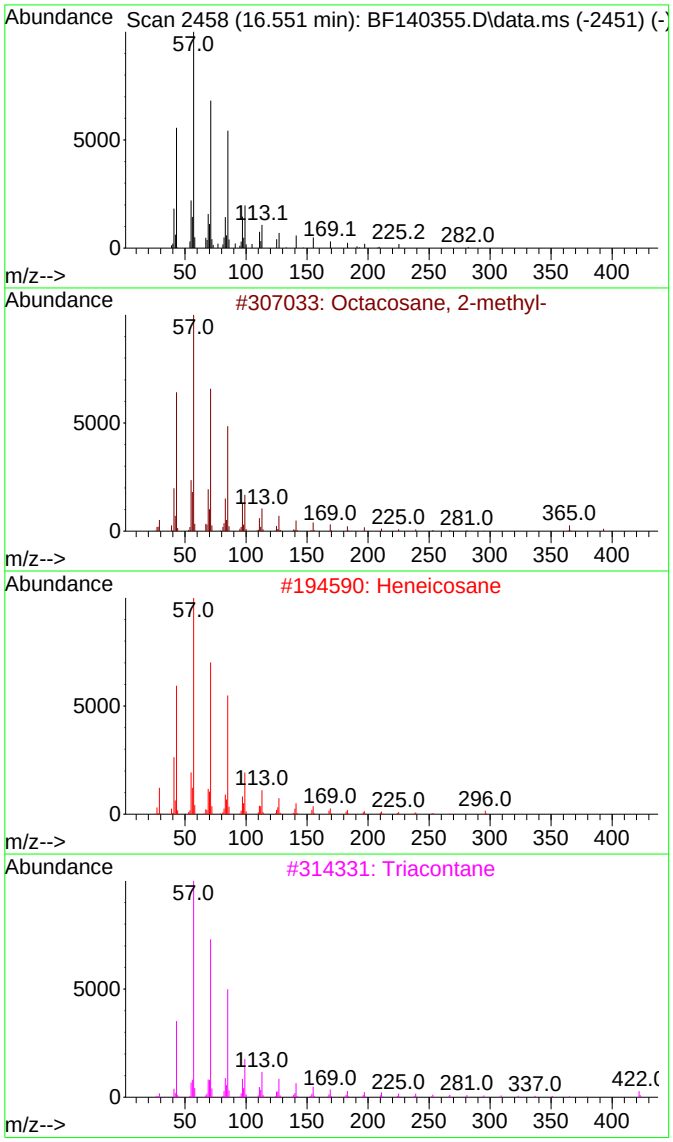
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

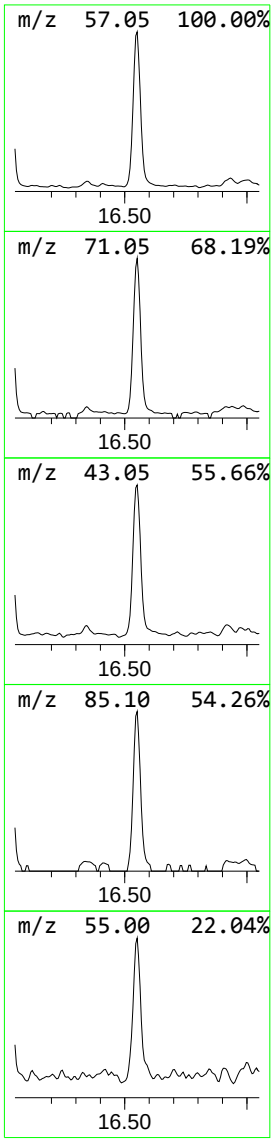
****

Peak Number 6 Octacosane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.551	2.22 ng	90473	Perylene-d12	15.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Triacontane	422	C30H62	000638-68-6	91
4	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
5	Tetratetracontane	619	C44H90	007098-22-8	90





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

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
2-Pentanone, 4-...	5.110	45.4	ng	1967480	1	6.875	866954	20.0
2-Cyclohexen-1-ol	5.687	3.6	ng	156579	1	6.875	866954	20.0
2-Cyclohexen-1-one	6.128	5.8	ng	251122	1	6.875	866954	20.0
2-Chlorocyclohe...	7.028	5.4	ng	233135	1	6.875	866954	20.0
Octacosane, 2-m...	16.551	2.2	ng	90473	6	15.557	816675	20.0