LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_E\Data\BE111324\
Data File : BE101595.D
Acq On : 13 Nov 2024 14:56
Operator : RC/JU
Sample : P4811-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_E
ClientSampleId :
RB24008

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_E\Methods\8270-BE110624.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BE101595.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.653	8	11	18	rVB	110003	153215	7.51%	1.448%
2	5.302	458	462	471	rVB	53161	89073	4.37%	0.842%
3	6.936	735	740	757	rVB	94307	201055	9.86%	1.900%
4	7.547	839	844	854	rVB	90897	151481	7.43%	1.432%
5	8.757	1044	1050	1070	rBV	206089	428843	21.03%	4.053%
6	10.314	1309	1315	1329	rVB	186400	358702	17.59%	3.390%
7	12.241	1637	1643	1649	rBV10	44793	112452	5.51%	1.063%
8	12.494	1682	1686	1690	rBV3	57134	85152	4.18%	0.805%
9	12.553	1692	1696	1705	rVV4	59476	132635	6.50%	1.254%
10	12.782	1728	1735	1742	rBV	905787	1583490	77.65%	14.966%
11	12.852	1743	1747	1752	rBV5	155072	280975	13.78%	2.656%
12	13.851	1914	1917	1921	rBV	992928	1684445	82.60%	15.920%
13	21.102	3148	3151	3161	rVB2	806118	1374605	67.41%	12.991%
14	21.578	3229	3232	3236	rVB2	133057	153725	7.54%	1.453%
15	21.977	3295	3300	3305	rBV	1476586	2039163	100.00%	19.272%
16	22.018	3305	3307	3319	rVB	154824	195856	9.60%	1.851%
17	22.312	3354	3357	3368	rVB	85193	125012	6.13%	1.181%
18	22.641	3409	3413	3418	rBV	81901	178727	8.76%	1.689%
19	22.823	3441	3444	3454	rVB2	51905	84690	4.15%	0.800%
20	23.140	3494	3498	3506	rVB	63294	120446	5.91%	1.138%
21	23.346	3526	3533	3540	rBV	481962	1047067	51.35%	9.896%

Sum of corrected areas: 10580809

Data Path : Z:\svoasrv\HPCHEM1\BNA_E\Data\BE111324\
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Misc :
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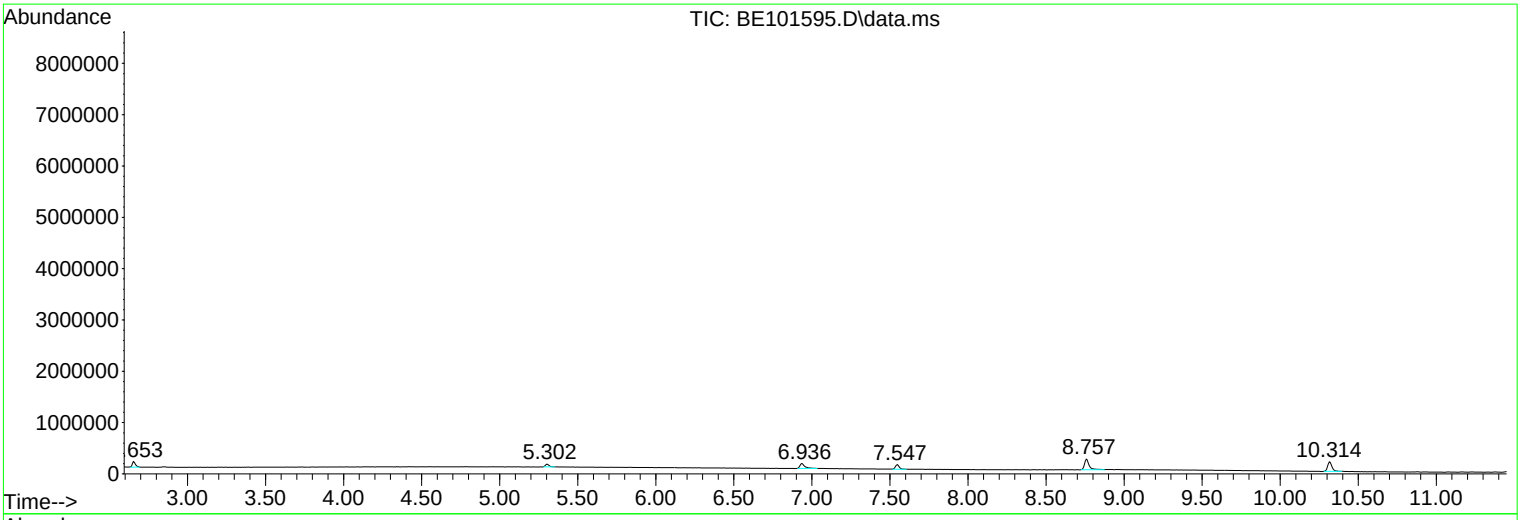
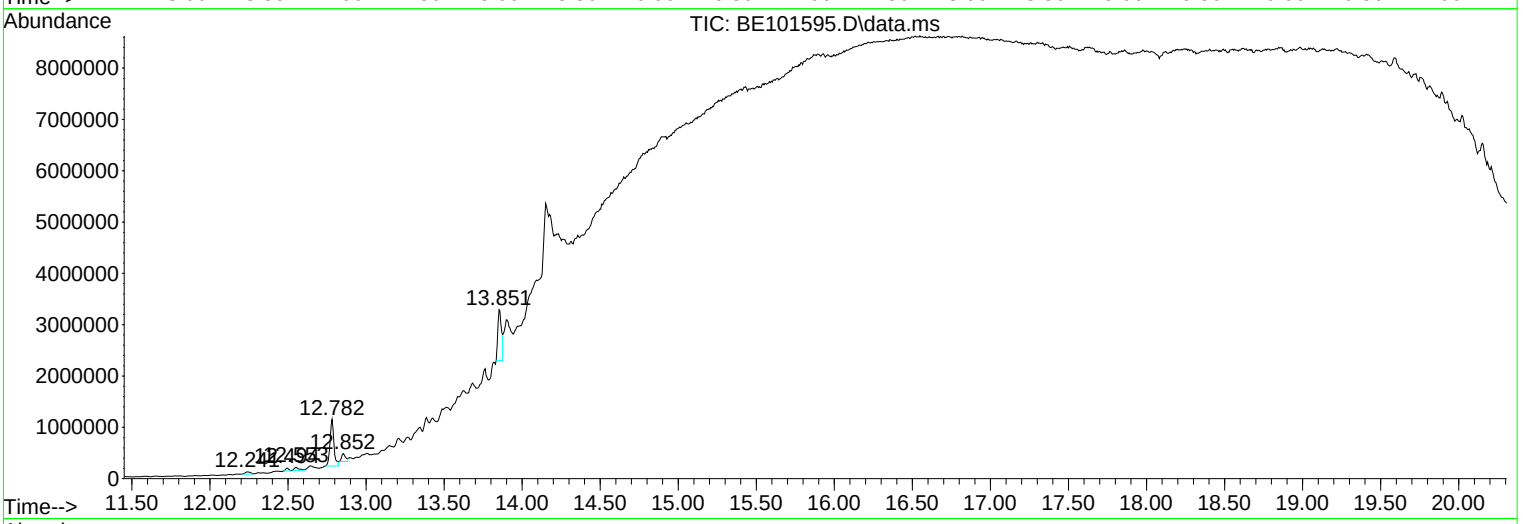
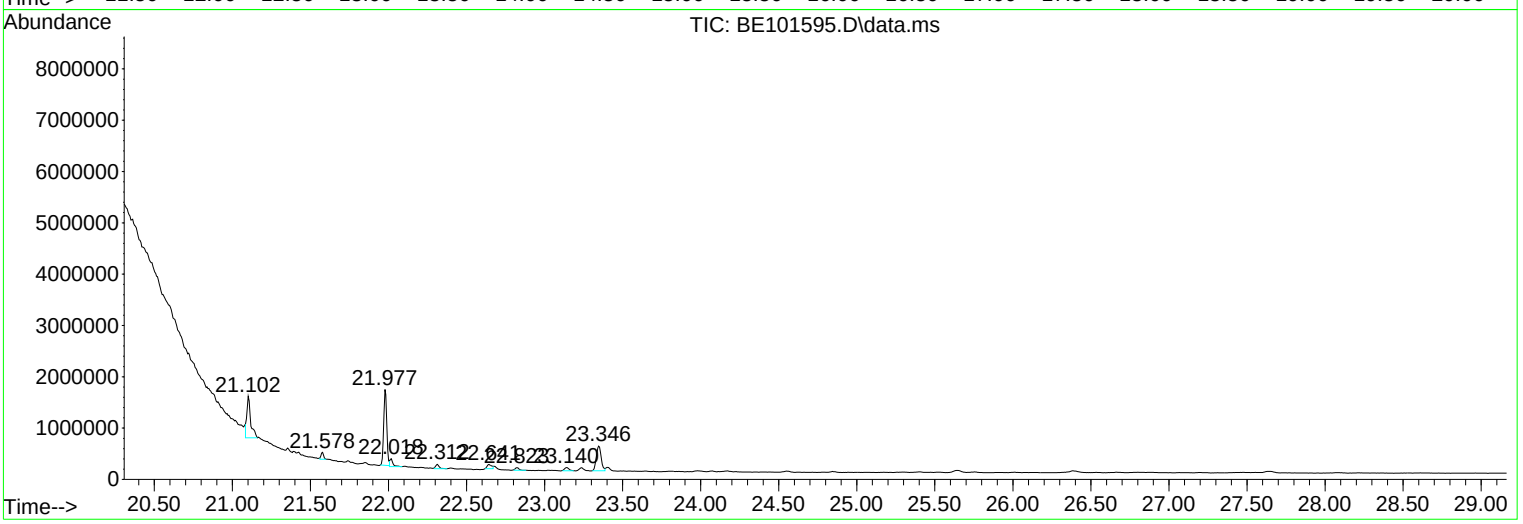
Instrument :
BNA_E
ClientSampleId :
RB24008

Quant Method : Z:\svoasrv\HPCHEM1\BNA_E\Methods\8270-BE110624.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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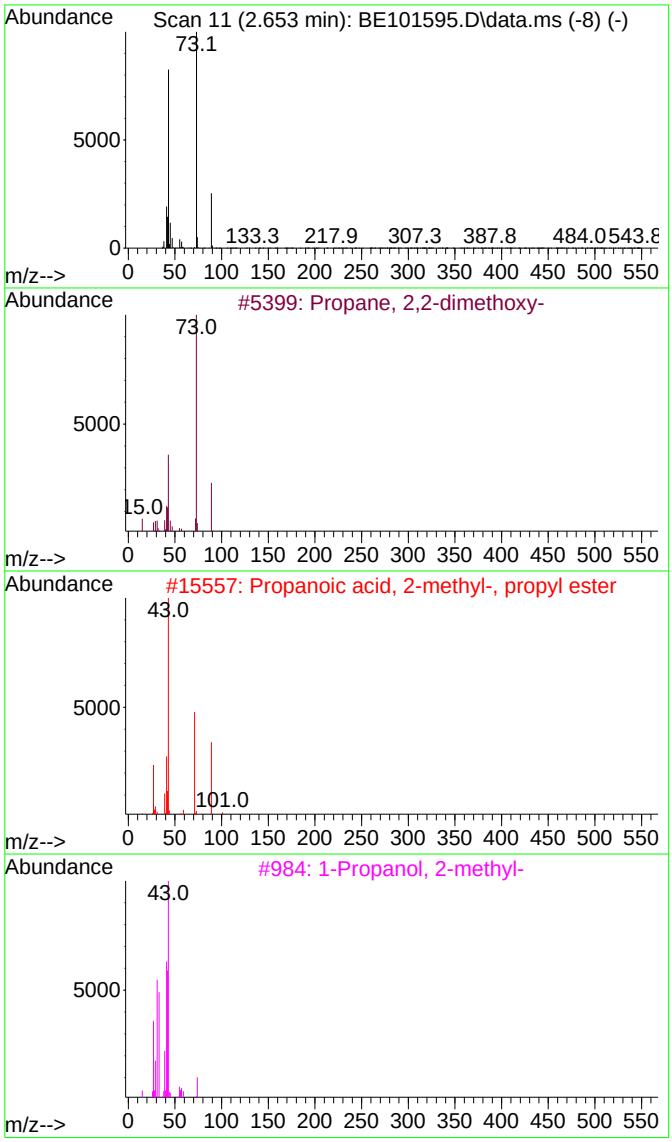
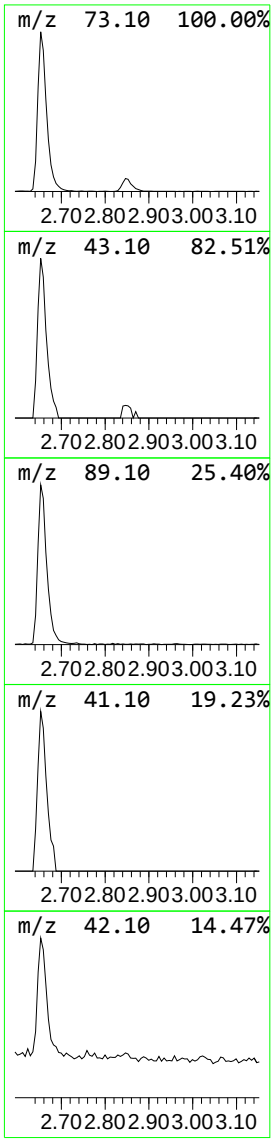
****

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.653	20.23 ng	153215	1,4-Dichlorobenzene-d4	7.547

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	64
2	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	25
3	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
4	Propyl nitrite	89	C3H7NO2	000543-67-9	9
5	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9





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Sample : P4811-01
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ALS Vial : 4 Sample Multiplier: 1

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BNA_E
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_E\Methods\8270-BE110624.M
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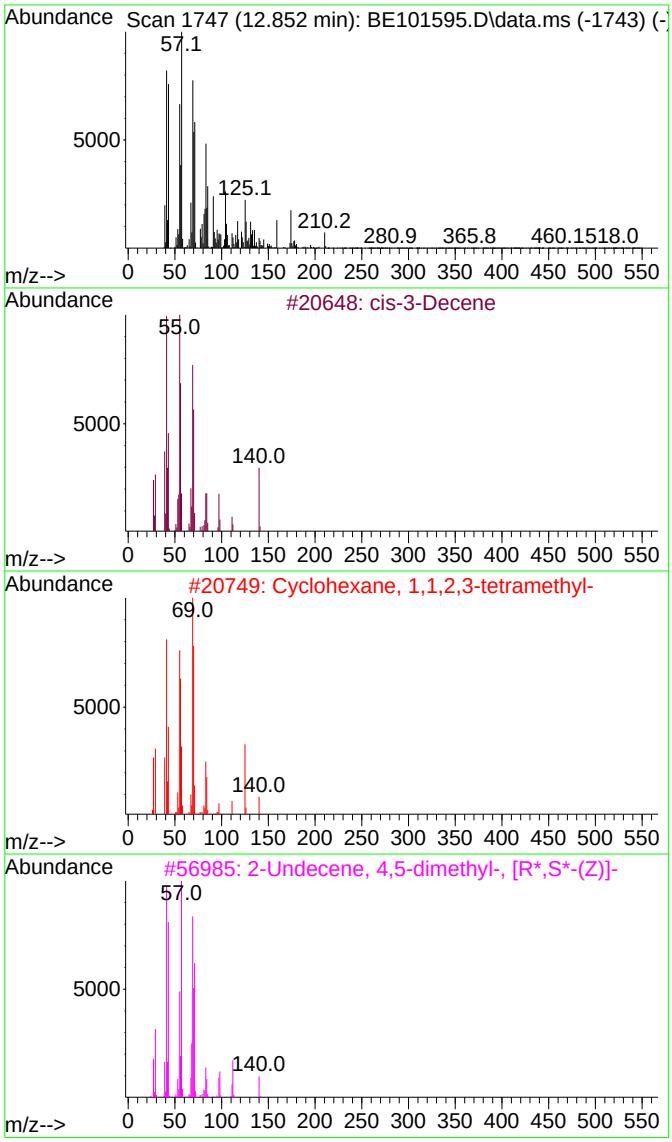
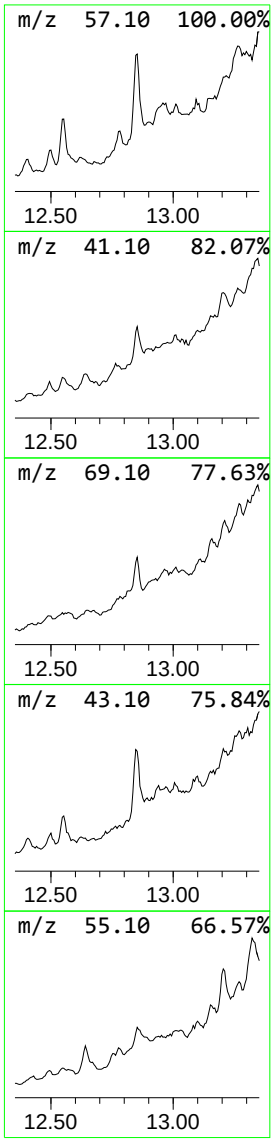
****

Peak Number 2 cis-3-Decene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.852	3.34 ng	280975	Acenaphthene-d10	14.169

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-3-Decene	140	C10H20	019398-86-8	55
2	Cyclohexane, 1,1,2,3-tetramethyl-	140	C10H20	006783-92-2	49
3	2-Undecene, 4,5-dimethyl-, [R*,S...	182	C13H26	055170-93-9	46
4	2-Octene, 2,6-dimethyl-	140	C10H20	004057-42-5	43
5	Formic acid, 2-ethylbutyl ester	130	C7H14O2	1000367-92-2	43





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Misc :
ALS Vial : 4 Sample Multiplier: 1

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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_E\Methods\8270-BE110624.M
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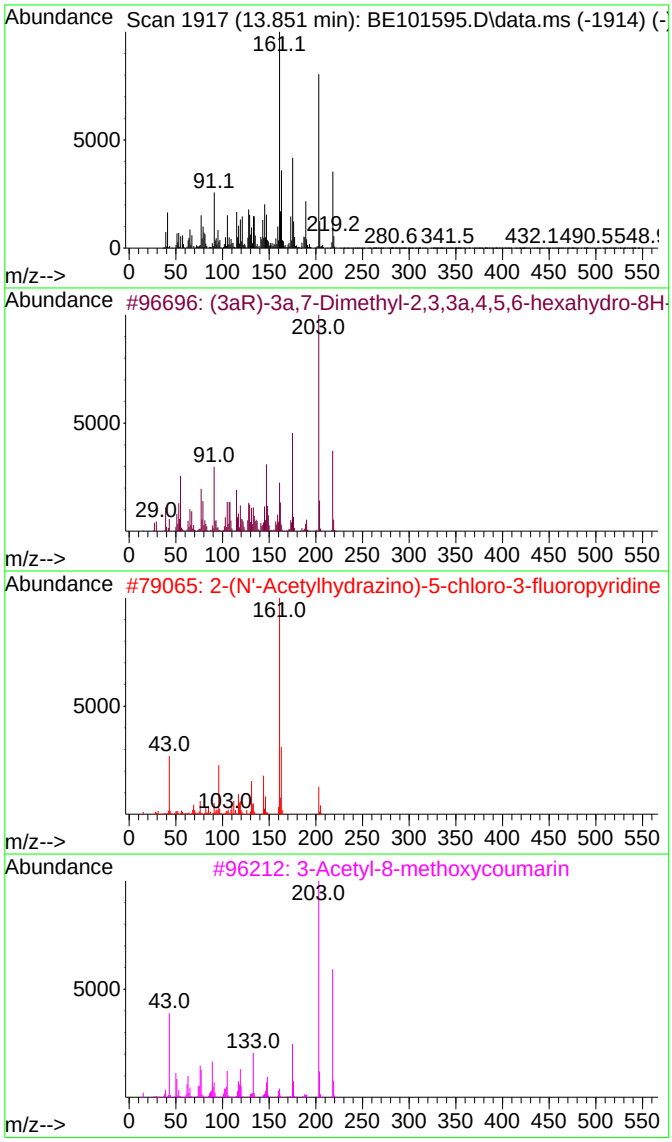
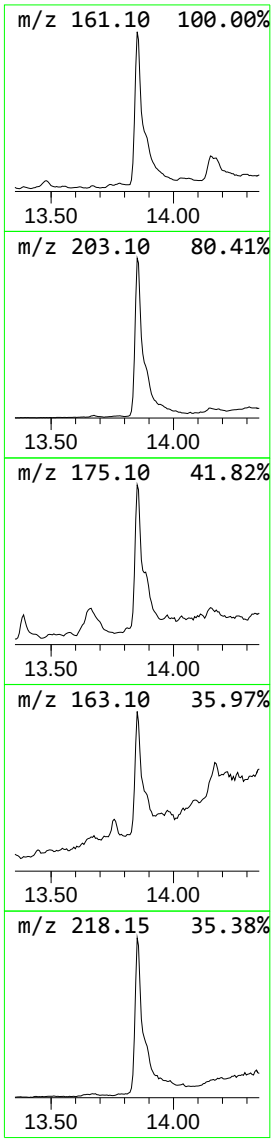
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 (3aR)-3a,7-Dimethyl-2,3,3a,... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.851	20.00 ng	1684450	Acenaphthene-d10	14.169

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(3aR)-3a,7-Dimethyl-2,3,3a,4,5,6...	218	C14H18O2	1000482-61-7	70
2	2-(N'-Acetylhydrazino)-5-chloro-...	203	C7H7ClFN3O	1150561-82-2	53
3	3-Acetyl-8-methoxycoumarin	218	C12H10O4	005452-39-1	49
4	Tetracyclo[6.1.0.0(2,4).0(5,7)]n...	204	C15H24	051898-92-1	38
5	4(3H)-Quinazolinone, 7-amino-3-e...	189	C10H11N3O	1000338-19-9	38





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Data File : BE101595.D
Acq On : 13 Nov 2024 14:56
Operator : RC/JU
Sample : P4811-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_E
ClientSampleId :
RB24008

Quant Method : Z:\svoasrv\HPCHEM1\BNA_E\Methods\8270-BE110624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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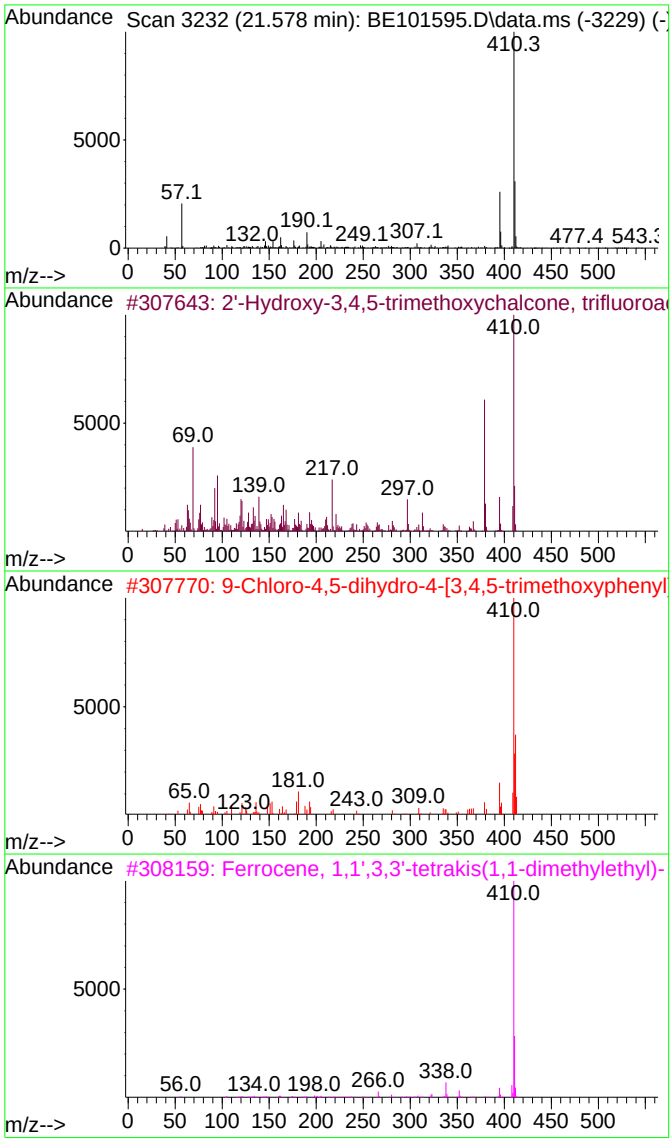
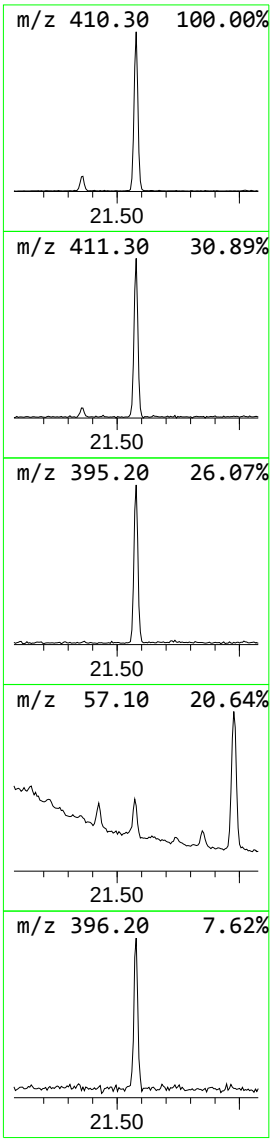
****
Peak Number 4 2'-Hydroxy-3,4,5-trimethoxy... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.578	2.24 ng	153725	Chrysene-d12	21.102

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2'-Hydroxy-3,4,5-trimethoxychalc...	410	C20H17F3O6	1000449-43-8	56
2	9-Chloro-4,5-dihydro-4-[3,4,5-tr...	410	C22H19ClN2O4	1000212-48-1	50
3	Ferrocene, 1,1',3,3'-tetrakis(1,...	410	C26H42Fe	001317-17-5	45
4	5-[(2-Hydroxyethyl)octadecylamin...	441	C27H55NO3	1010185-08-9	45
5	Di(trimethylene-1-naphthyl)siloxane	410	C26H26OSi2	093241-94-2	43





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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_E\Methods\8270-BE110624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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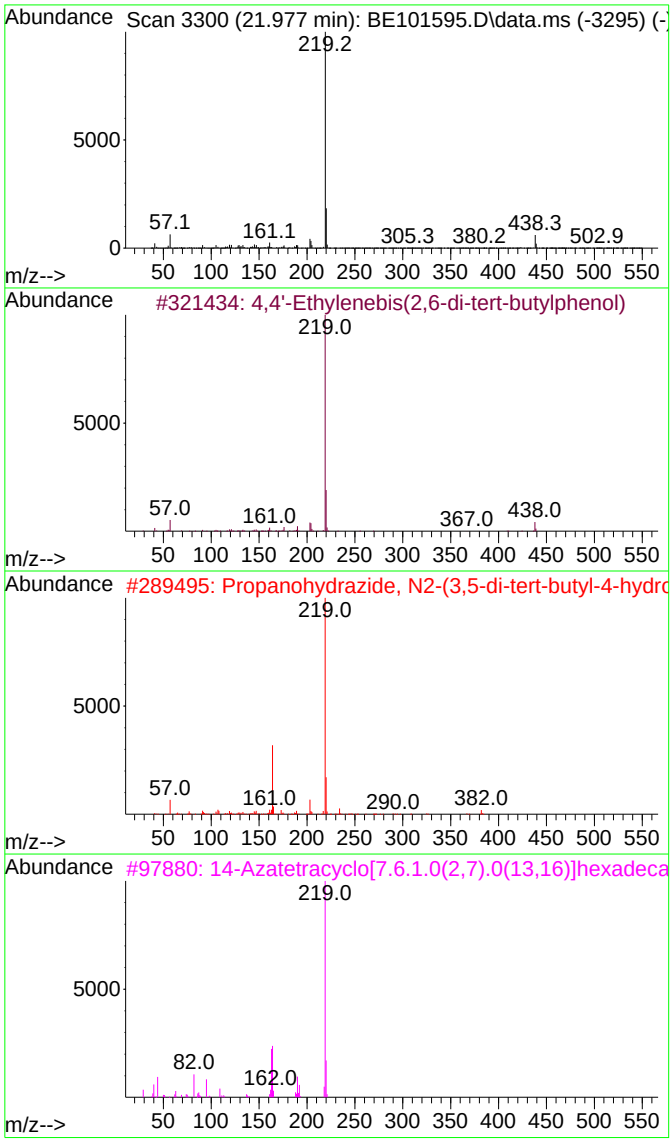
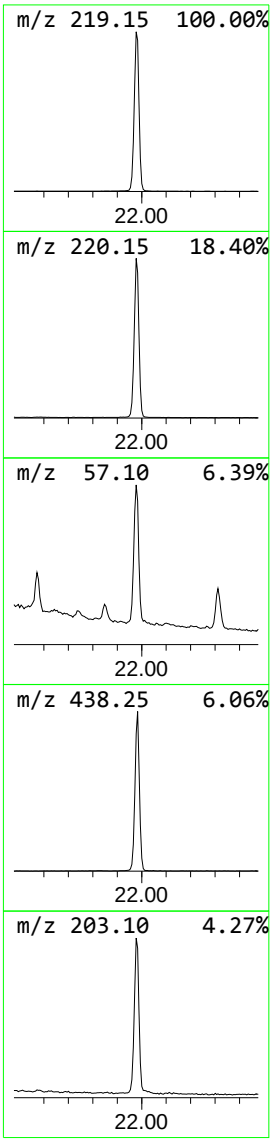
****
Peak Number 5 4,4'-Ethylenebis(2,6-di-ter... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.977	29.67 ng	2039160	Chrysene-d12	21.102

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,4'-Ethylenebis(2,6-di-tert-but...	438	C30H46O2	001516-94-5	94
2	Propanohydrazide, N2-(3,5-di-ter...	382	C24H34N2O2	304870-86-8	72
3	14-Azatetracyclo[7.6.1.0(2,7).0(...	219	C15H9NO	042326-31-8	72
4	2-Methyl-4-phenylquinoline	219	C16H13N	001721-92-2	72
5	3,5-di-tert-Butyl-4-hydroxybenza...	234	C15H22O2	001620-98-0	64





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_E\Methods\8270-BE110624.M
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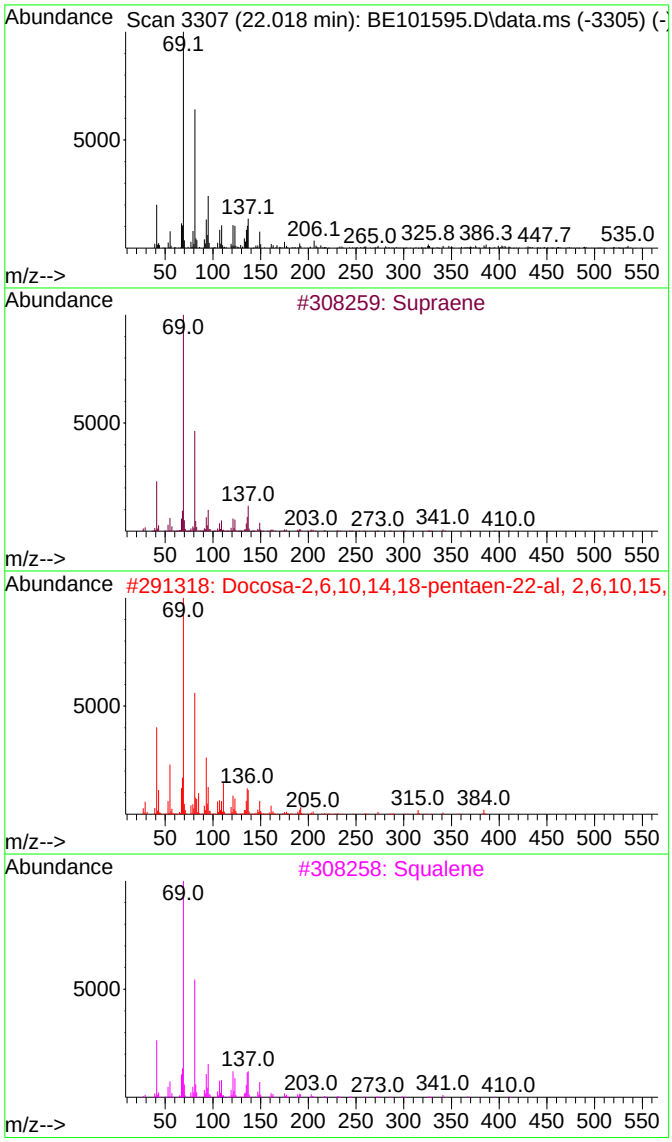
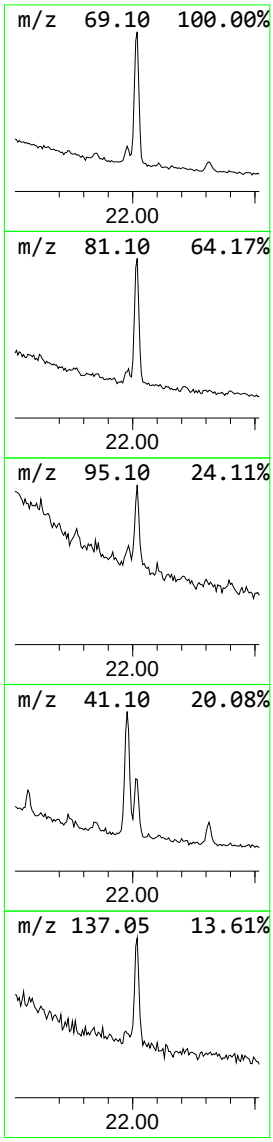
****

Peak Number 6 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.018	2.85 ng	195856	Chrysene-d12	21.102

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	89
2	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	89
3	Squalene	410	C30H50	000111-02-4	76
4	2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	74
5	2-Octene, 2-methyl-6-methylene-	138	C10H18	010054-09-8	64





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Sample : P4811-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_E\Methods\8270-BE110624.M
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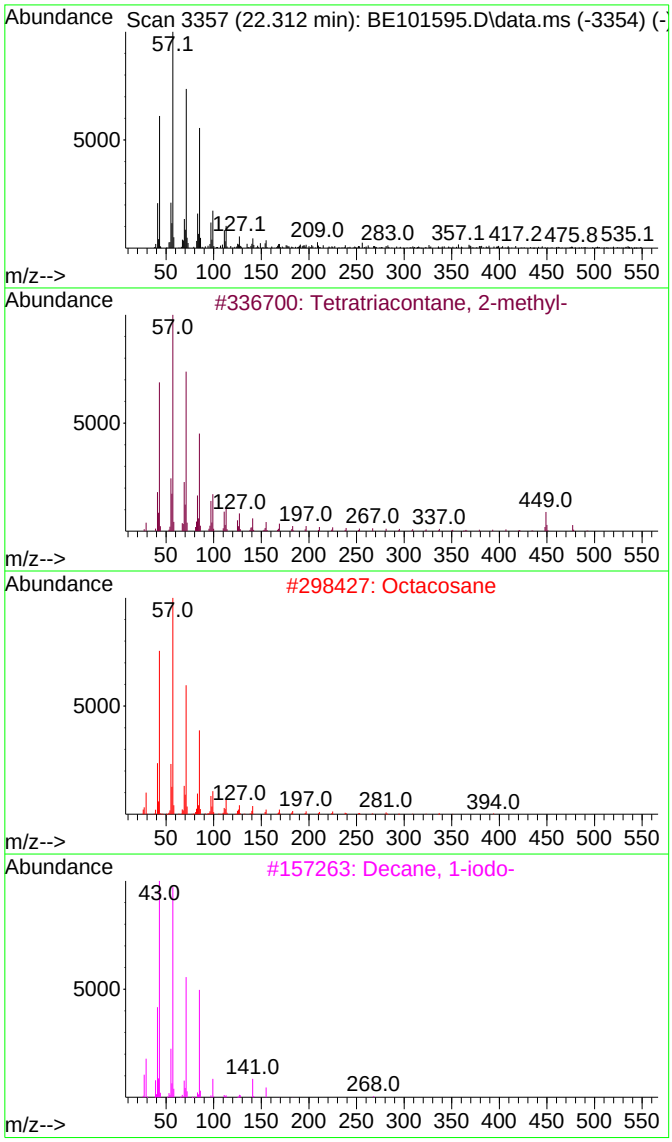
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

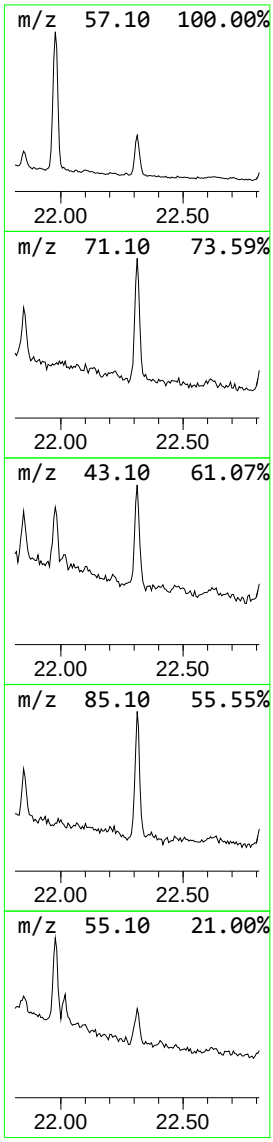
****

Peak Number 7 Tetratriacontane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.312	2.39 ng	125012	Perylene-d12	23.346

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratriacontane, 2-methyl-	493	C35H72	014167-65-8	93
2	Octacosane	394	C28H58	000630-02-4	91
3	Decane, 1-iodo-	268	C10H21I	002050-77-3	87
4	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	87
5	Heneicosane	296	C21H44	000629-94-7	83





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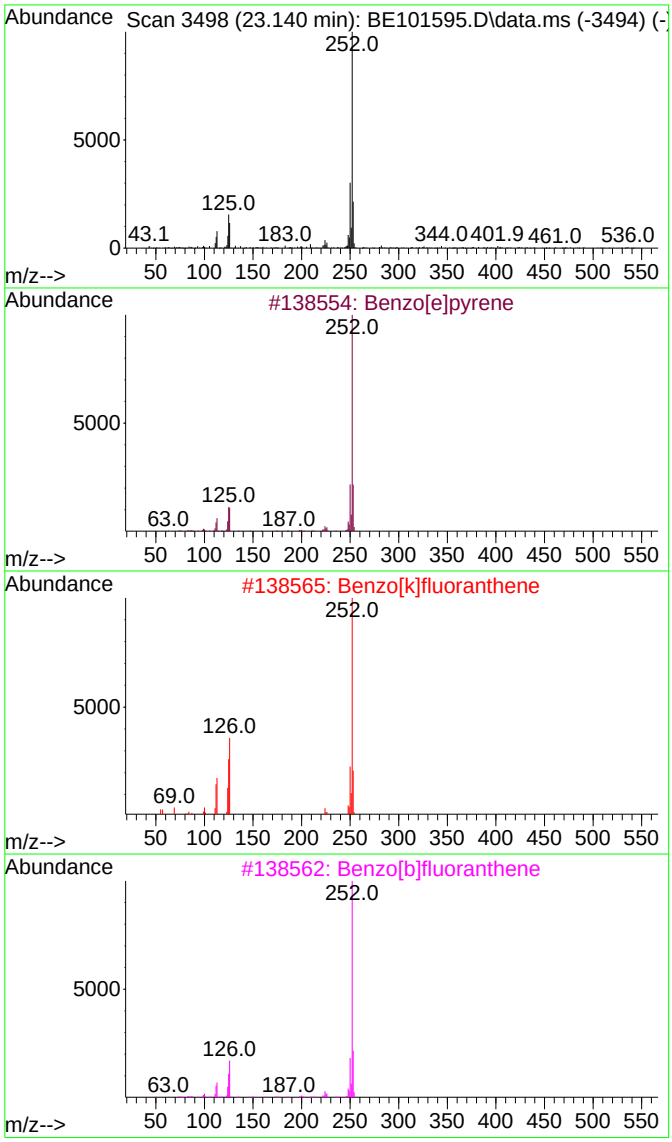
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

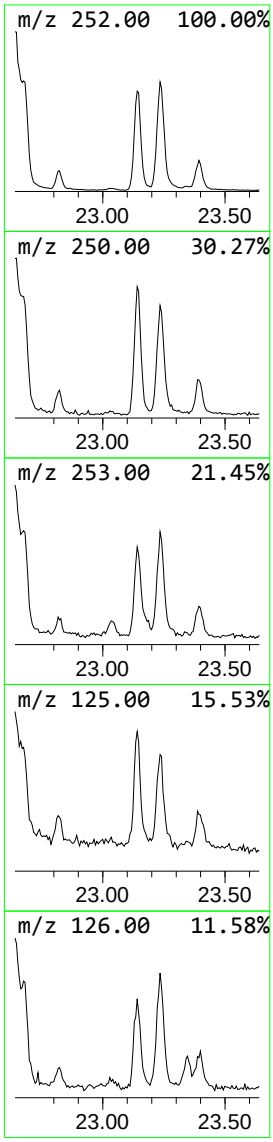
****

Peak Number 8 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.140	2.30 ng	120446	Perylene-d12	23.346

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	95
4	Benzo[j]fluoranthene	252	C20H12	000205-82-3	94
5	Benzo[a]pyrene	252	C20H12	000050-32-8	93





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
Propane, 2,2-di...	2.653	20.2	ng	153215	1	7.547	151481	20.0
cis-3-Decene	12.852	3.3	ng	280975	3	14.169	1684450	20.0
(3aR)-3a,7-Dime...	13.851	20.0	ng	1684450	3	14.169	1684450	20.0
2'-Hydroxy-3,4,...	21.578	2.2	ng	153725	5	21.102	1374610	20.0
4,4'-Ethylenebi...	21.977	29.7	ng	2039160	5	21.102	1374610	20.0
Supraene	22.018	2.9	ng	195856	5	21.102	1374610	20.0
Tetratriacontan...	22.312	2.4	ng	125012	6	23.346	1047070	20.0
Benzo[e]pyrene	23.140	2.3	ng	120446	6	23.346	1047070	20.0